Norditerpenoid Alkaloids from Medicinal Plants

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Award date:
2020

Awarding institution:
University of Bath

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Volume 2 of 2

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A thesis submitted for the degree of Doctor of Philosophy

University of Bath

Department of Pharmacy and Pharmacology

September 2019

Signed ……

Date …….

Appendix II: Data of single-crystal X-ray determinations

Contents

s17phar5: ethyl (1*S*,5*S*,*E*)-9-(2-(2,4-dinitrophenyl)hydrazinylidene)-3-ethyl-3-azabicyclo[3.3.1] nonane-1-carboxylate (**15**)

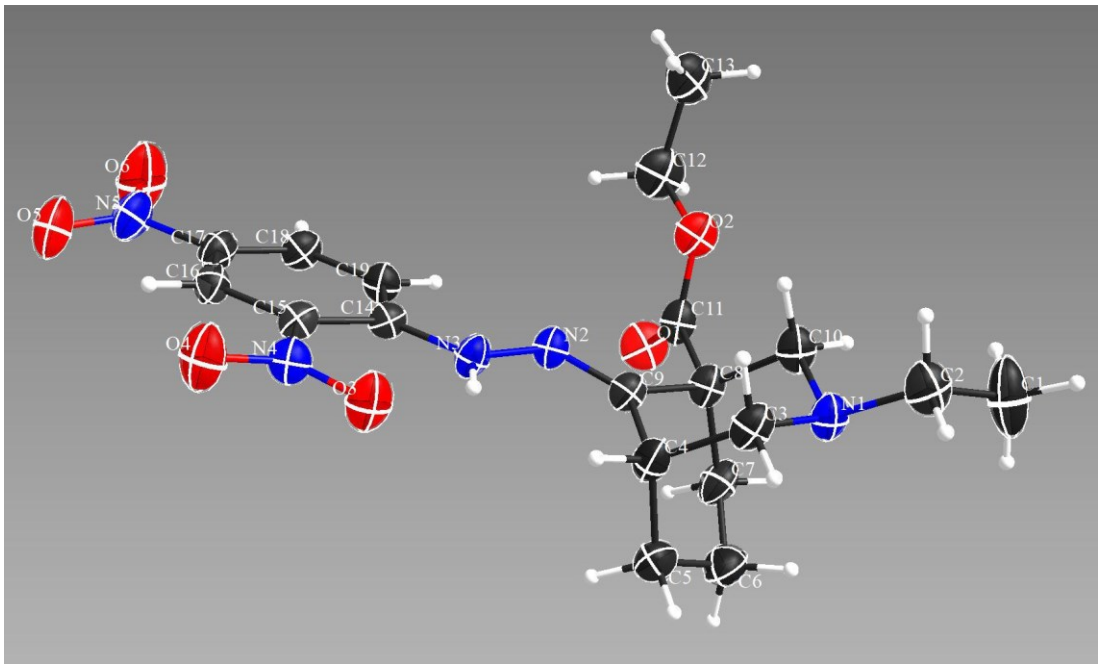

Table 1. Crystal data and structure refinement for s17phar5.

Identification code	s17phar5	
Empirical formula	C19 H25 N5 O6	
Formula weight	419.44	
Temperature	150.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	I2/a	
Unit cell dimensions	a = 26.8708(18) Å	α= 90°.
	b = 7.3323(7) Å	β= 95.548(6)°.
	c = 20.6528(14) Å	γ = 90°.
Volume	4050.1(5) Å^3	
Z	8	
Density (calculated)	1.376 Mg/m^3	
Absorption coefficient	0.872 mm^{-1}	
F(000)	1776	
Crystal size	0.100 x 0.080 x 0.020 mm^3	
Theta range for data collection	3.305 to 73.477°.	
Index ranges	-33<=h<=31, -7<=k<=8, -22<=l<=25	

Reflections collected	13152
Independent reflections	4023 [R(int) = 0.0446]
Completeness to theta = 67.684°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.84944
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4023 / 0 / 277
Goodness-of-fit on F^2	1.020
Final R indices [I>2sigma(I)]	R1 = 0.0537, wR2 = 0.1391
R indices (all data)	R1 = 0.0744, wR2 = 0.1534
Extinction coefficient	n/a
Largest diff. peak and hole	0.421 and -0.227 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for s17phar5. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	3387(1)	2649(3)	4907(1)	46(1)
C(1)	5591(1)	4766(5)	5896(1)	63(1)
N(1)	4925(1)	2878(3)	6320(1)	32(1)
O(2)	3577(1)	5035(2)	5554(1)	38(1)
C(2)	5342(1)	4114(4)	6485(1)	40(1)
N(2)	3445(1)	1639(2)	6401(1)	28(1)
O(3)	3384(1)	-704(3)	8088(1)	42(1)
C(3)	4762(1)	2023(3)	6904(1)	33(1)
N(3)	3287(1)	801(3)	6944(1)	29(1)
N(4)	2926(1)	-745(3)	8113(1)	31(1)
O(4)	2738(1)	-1327(3)	8587(1)	47(1)
C(4)	4335(1)	657(3)	6743(1)	33(1)
O(5)	1091(1)	-765(3)	7604(1)	50(1)
C(5)	4484(1)	-1010(3)	6351(1)	43(1)
N(5)	1227(1)	124(3)	7151(1)	43(1)
C(9)	3912(1)	1574(3)	6334(1)	27(1)
C(8)	4092(1)	2418(3)	5728(1)	29(1)
C(7)	4281(1)	844(3)	5314(1)	39(1)
O(6)	939(1)	847(4)	6738(1)	73(1)
C(6)	4636(1)	-518(4)	5684(1)	44(1)

C(10)	4503(1)	3791(3)	5954(1)	33(1)
C(11)	3649(1)	3349(3)	5343(1)	33(1)
C(12)	3119(1)	5921(4)	5280(1)	50(1)
C(13)	3114(1)	7796(4)	5564(2)	53(1)
C(14)	2793(1)	649(3)	7001(1)	26(1)
C(15)	2602(1)	-103(3)	7560(1)	27(1)
C(16)	2090(1)	-268(3)	7606(1)	29(1)
C(17)	1763(1)	312(3)	7099(1)	31(1)
C(18)	1931(1)	1076(3)	6540(1)	32(1)
C(19)	2435(1)	1236(3)	6492(1)	30(1)

Table 3. Bond lengths [Å] for s17phar5.

O(1)-C(11)	1.203(3)
C(1)-C(2)	1.521(4)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
N(1)-C(2)	1.455(3)
N(1)-C(10)	1.463(3)
N(1)-C(3)	1.464(3)
O(2)-C(11)	1.331(3)
O(2)-C(12)	1.457(3)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
N(2)-C(9)	1.277(3)
N(2)-N(3)	1.382(2)
O(3)-N(4)	1.238(2)
C(3)-C(4)	1.535(3)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
N(3)-C(14)	1.349(3)
N(3)-H(3)	0.85(3)
N(4)-O(4)	1.221(2)
N(4)-C(15)	1.447(3)
C(4)-C(9)	1.506(3)
C(4)-C(5)	1.541(3)

C(4)-H(4)	1.0000
O(5)-N(5)	1.225(3)
C(5)-C(6)	1.518(4)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
N(5)-O(6)	1.218(3)
N(5)-C(17)	1.462(3)
C(9)-C(8)	1.516(3)
C(8)-C(11)	1.527(3)
C(8)-C(10)	1.534(3)
C(8)-C(7)	1.551(3)
C(7)-C(6)	1.534(4)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(12)-C(13)	1.495(4)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-C(15)	1.419(3)
C(14)-C(19)	1.421(3)
C(15)-C(16)	1.394(3)
C(16)-C(17)	1.367(3)
C(16)-H(16)	0.9500
C(17)-C(18)	1.397(3)
C(18)-C(19)	1.372(3)
C(18)-H(18)	0.9500
C(19)-H(19)	0.9500

Table 4. Bond angles [°] for s17phar5.

C(2)-C(1)-H(1A)	109.5

C(2)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(2)-N(1)-C(10)	112.12(18)
C(2)-N(1)-C(3)	110.98(17)
C(10)-N(1)-C(3)	110.00(17)
C(11)-O(2)-C(12)	115.50(18)
N(1)-C(2)-C(1)	113.3(2)
N(1)-C(2)-H(2A)	108.9
C(1)-C(2)-H(2A)	108.9
N(1)-C(2)-H(2B)	108.9
C(1)-C(2)-H(2B)	108.9
H(2A)-C(2)-H(2B)	107.7
C(9)-N(2)-N(3)	116.98(18)
N(1)-C(3)-C(4)	112.25(17)
N(1)-C(3)-H(3A)	109.2
C(4)-C(3)-H(3A)	109.2
N(1)-C(3)-H(3B)	109.2
C(4)-C(3)-H(3B)	109.2
H(3A)-C(3)-H(3B)	107.9
C(14)-N(3)-N(2)	119.30(18)
C(14)-N(3)-H(3)	117.9(17)
N(2)-N(3)-H(3)	122.7(17)
O(4)-N(4)-O(3)	122.20(19)
O(4)-N(4)-C(15)	118.88(18)
O(3)-N(4)-C(15)	118.91(18)
C(9)-C(4)-C(3)	109.71(18)
C(9)-C(4)-C(5)	106.23(19)
C(3)-C(4)-C(5)	113.84(19)
C(9)-C(4)-H(4)	109.0
C(3)-C(4)-H(4)	109.0
C(5)-C(4)-H(4)	109.0
C(6)-C(5)-C(4)	113.3(2)
C(6)-C(5)-H(5A)	108.9
C(4)-C(5)-H(5A)	108.9
C(6)-C(5)-H(5B)	108.9
C(4)-C(5)-H(5B)	108.9

H(5A)-C(5)-H(5B)	107.7
O(6)-N(5)-O(5)	123.4(2)
O(6)-N(5)-C(17)	118.2(2)
O(5)-N(5)-C(17)	118.4(2)
N(2)-C(9)-C(4)	130.68(19)
N(2)-C(9)-C(8)	117.92(18)
C(4)-C(9)-C(8)	111.25(17)
C(9)-C(8)-C(11)	108.62(17)
C(9)-C(8)-C(10)	107.15(17)
C(11)-C(8)-C(10)	111.54(18)
C(9)-C(8)-C(7)	107.38(18)
C(11)-C(8)-C(7)	108.96(18)
C(10)-C(8)-C(7)	113.01(18)
C(6)-C(7)-C(8)	115.53(19)
C(6)-C(7)-H(7A)	108.4
C(8)-C(7)-H(7A)	108.4
C(6)-C(7)-H(7B)	108.4
C(8)-C(7)-H(7B)	108.4
H(7A)-C(7)-H(7B)	107.5
C(5)-C(6)-C(7)	113.4(2)
C(5)-C(6)-H(6A)	108.9
C(7)-C(6)-H(6A)	108.9
C(5)-C(6)-H(6B)	108.9
C(7)-C(6)-H(6B)	108.9
H(6A)-C(6)-H(6B)	107.7
N(1)-C(10)-C(8)	110.88(18)
N(1)-C(10)-H(10A)	109.5
C(8)-C(10)-H(10A)	109.5
N(1)-C(10)-H(10B)	109.5
C(8)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	108.1
O(1)-C(11)-O(2)	123.3(2)
O(1)-C(11)-C(8)	124.7(2)
O(2)-C(11)-C(8)	112.00(18)
O(2)-C(12)-C(13)	107.2(2)
O(2)-C(12)-H(12A)	110.3
C(13)-C(12)-H(12A)	110.3
O(2)-C(12)-H(12B)	110.3
C(13)-C(12)-H(12B)	110.3

H(12A)-C(12)-H(12B)	108.5
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
N(3)-C(14)-C(15)	122.55(19)
N(3)-C(14)-C(19)	120.84(19)
C(15)-C(14)-C(19)	116.61(19)
C(16)-C(15)-C(14)	121.72(19)
C(16)-C(15)-N(4)	116.14(19)
C(14)-C(15)-N(4)	122.14(18)
C(17)-C(16)-C(15)	119.0(2)
C(17)-C(16)-H(16)	120.5
C(15)-C(16)-H(16)	120.5
C(16)-C(17)-C(18)	121.6(2)
C(16)-C(17)-N(5)	118.6(2)
C(18)-C(17)-N(5)	119.8(2)
C(19)-C(18)-C(17)	119.5(2)
C(19)-C(18)-H(18)	120.2
C(17)-C(18)-H(18)	120.2
C(18)-C(19)-C(14)	121.5(2)
C(18)-C(19)-H(19)	119.2
C(14)-C(19)-H(19)	119.2

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for s17phar5. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	44(1)	59(1)	32(1)	-6(1)	-14(1)	-2(1)
C(1)	47(2)	90(2)	49(2)	20(2)	-11(1)	-32(2)
N(1)	26(1)	40(1)	30(1)	6(1)	-2(1)	-2(1)
O(2)	29(1)	45(1)	36(1)	2(1)	-10(1)	2(1)
C(2)	37(1)	46(1)	36(1)	4(1)	-8(1)	-5(1)

N(2)	27(1)	35(1)	23(1)	1(1)	2(1)	-2(1)
O(3)	27(1)	59(1)	37(1)	11(1)	-3(1)	1(1)
C(3)	26(1)	44(1)	27(1)	4(1)	-2(1)	4(1)
N(3)	24(1)	38(1)	26(1)	3(1)	2(1)	1(1)
N(4)	32(1)	36(1)	25(1)	1(1)	0(1)	-1(1)
O(4)	42(1)	71(1)	26(1)	13(1)	3(1)	-3(1)
C(4)	26(1)	41(1)	32(1)	9(1)	6(1)	4(1)
O(5)	33(1)	75(1)	45(1)	1(1)	12(1)	-10(1)
C(5)	32(1)	37(1)	60(2)	4(1)	3(1)	4(1)
N(5)	26(1)	57(1)	46(1)	-2(1)	4(1)	0(1)
C(9)	25(1)	33(1)	24(1)	-1(1)	0(1)	0(1)
C(8)	26(1)	39(1)	23(1)	1(1)	0(1)	-1(1)
C(7)	33(1)	52(2)	32(1)	-8(1)	7(1)	1(1)
O(6)	27(1)	112(2)	78(2)	34(1)	-2(1)	8(1)
C(6)	38(1)	43(1)	53(2)	-10(1)	12(1)	1(1)
C(10)	29(1)	40(1)	28(1)	7(1)	-3(1)	-4(1)
C(11)	28(1)	46(1)	23(1)	4(1)	0(1)	-4(1)
C(12)	35(1)	58(2)	53(2)	2(1)	-16(1)	5(1)
C(13)	37(1)	50(2)	71(2)	6(1)	-9(1)	1(1)
C(14)	25(1)	28(1)	25(1)	-2(1)	1(1)	1(1)
C(15)	26(1)	31(1)	23(1)	-3(1)	0(1)	2(1)
C(16)	29(1)	32(1)	27(1)	-2(1)	6(1)	-3(1)
C(17)	22(1)	37(1)	36(1)	-4(1)	3(1)	0(1)
C(18)	26(1)	37(1)	32(1)	1(1)	-3(1)	3(1)
C(19)	29(1)	34(1)	27(1)	4(1)	1(1)	0(1)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3)

for s17phar5.

	x	y	z	U(eq)
H(1A)	5889	5484	6042	95
H(1B)	5357	5524	5621	95
H(1C)	5689	3710	5647	95
H(2A)	5594	3488	6789	48
H(2B)	5220	5187	6714	48

H(3A)	4649	2982	7194	39
H(3B)	5049	1384	7140	39
H(3)	3488(10)	310(40)	7236(13)	36(7)
H(4)	4211	226	7158	40
H(5A)	4766	-1645	6600	52
H(5B)	4199	-1868	6297	52
H(7A)	3987	166	5112	47
H(7B)	4454	1383	4957	47
H(6A)	4649	-1645	5422	53
H(6B)	4977	9	5735	53
H(10A)	4620	4411	5571	39
H(10B)	4366	4729	6232	39
H(12A)	2824	5224	5391	60
H(12B)	3111	5989	4801	60
H(13A)	2788	8363	5445	80
H(13B)	3377	8533	5395	80
H(13C)	3175	7719	6039	80
H(16)	1969	-776	7984	35
H(18)	1698	1483	6195	38
H(19)	2547	1751	6110	36

Table 7. Torsion angles [°] for s17phar5.

C(10)-N(1)-C(2)-C(1)	-67.4(3)
C(3)-N(1)-C(2)-C(1)	169.1(2)
C(2)-N(1)-C(3)-C(4)	-177.91(19)
C(10)-N(1)-C(3)-C(4)	57.4(2)
C(9)-N(2)-N(3)-C(14)	-172.55(19)
N(1)-C(3)-C(4)-C(9)	-54.1(2)
N(1)-C(3)-C(4)-C(5)	64.8(3)
C(9)-C(4)-C(5)-C(6)	57.7(3)
C(3)-C(4)-C(5)-C(6)	-63.1(3)
N(3)-N(2)-C(9)-C(4)	2.6(3)
N(3)-N(2)-C(9)-C(8)	177.64(18)
C(3)-C(4)-C(9)-N(2)	-129.5(2)
C(5)-C(4)-C(9)-N(2)	107.0(3)

C(3)-C(4)-C(9)-C(8)	55.2(2)
C(5)-C(4)-C(9)-C(8)	-68.3(2)
N(2)-C(9)-C(8)-C(11)	5.0(3)
C(4)-C(9)-C(8)-C(11)	-179.04(18)
N(2)-C(9)-C(8)-C(10)	125.6(2)
C(4)-C(9)-C(8)-C(10)	-58.4(2)
N(2)-C(9)-C(8)-C(7)	-112.7(2)
C(4)-C(9)-C(8)-C(7)	63.3(2)
C(9)-C(8)-C(7)-C(6)	-48.3(3)
C(11)-C(8)-C(7)-C(6)	-165.7(2)
C(10)-C(8)-C(7)-C(6)	69.7(3)
C(4)-C(5)-C(6)-C(7)	-45.3(3)
C(8)-C(7)-C(6)-C(5)	40.8(3)
C(2)-N(1)-C(10)-C(8)	174.36(18)
C(3)-N(1)-C(10)-C(8)	-61.6(2)
C(9)-C(8)-C(10)-N(1)	61.5(2)
C(11)-C(8)-C(10)-N(1)	-179.71(17)
C(7)-C(8)-C(10)-N(1)	-56.5(2)
C(12)-O(2)-C(11)-O(1)	7.5(3)
C(12)-O(2)-C(11)-C(8)	-171.1(2)
C(9)-C(8)-C(11)-O(1)	-93.8(3)
C(10)-C(8)-C(11)-O(1)	148.4(2)
C(7)-C(8)-C(11)-O(1)	22.9(3)
C(9)-C(8)-C(11)-O(2)	84.8(2)
C(10)-C(8)-C(11)-O(2)	-33.0(2)
C(7)-C(8)-C(11)-O(2)	-158.49(19)
C(11)-O(2)-C(12)-C(13)	-178.7(2)
N(2)-N(3)-C(14)-C(15)	-176.47(19)
N(2)-N(3)-C(14)-C(19)	4.0(3)
N(3)-C(14)-C(15)-C(16)	-179.2(2)
C(19)-C(14)-C(15)-C(16)	0.4(3)
N(3)-C(14)-C(15)-N(4)	0.7(3)
C(19)-C(14)-C(15)-N(4)	-179.77(19)
O(4)-N(4)-C(15)-C(16)	-2.3(3)
O(3)-N(4)-C(15)-C(16)	177.0(2)
O(4)-N(4)-C(15)-C(14)	177.8(2)
O(3)-N(4)-C(15)-C(14)	-2.9(3)
C(14)-C(15)-C(16)-C(17)	-0.1(3)
N(4)-C(15)-C(16)-C(17)	-179.93(19)

C(15)-C(16)-C(17)-C(18)	-0.5(3)
C(15)-C(16)-C(17)-N(5)	179.7(2)
O(6)-N(5)-C(17)-C(16)	170.9(2)
O(5)-N(5)-C(17)-C(16)	-9.8(3)
O(6)-N(5)-C(17)-C(18)	-9.0(4)
O(5)-N(5)-C(17)-C(18)	170.4(2)
C(16)-C(17)-C(18)-C(19)	0.6(3)
N(5)-C(17)-C(18)-C(19)	-179.5(2)
C(17)-C(18)-C(19)-C(14)	-0.3(3)
N(3)-C(14)-C(19)-C(18)	179.4(2)
C(15)-C(14)-C(19)-C(18)	-0.2(3)

Table 8. Hydrogen bonds for s17phar5 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(3)-H(3)...O(3)	0.85(3)	1.95(3)	2.596(2)	132(2)

s17phar6: methyl (1*R*,5*R*,7*S*,*E*)-9-(2-(2,4-dinitrophenyl)hydrazinylidene)-3-ethyl-7-isopropyl-3-azabicyclo [3.3.1]nonane-1-carboxylate (**16**)

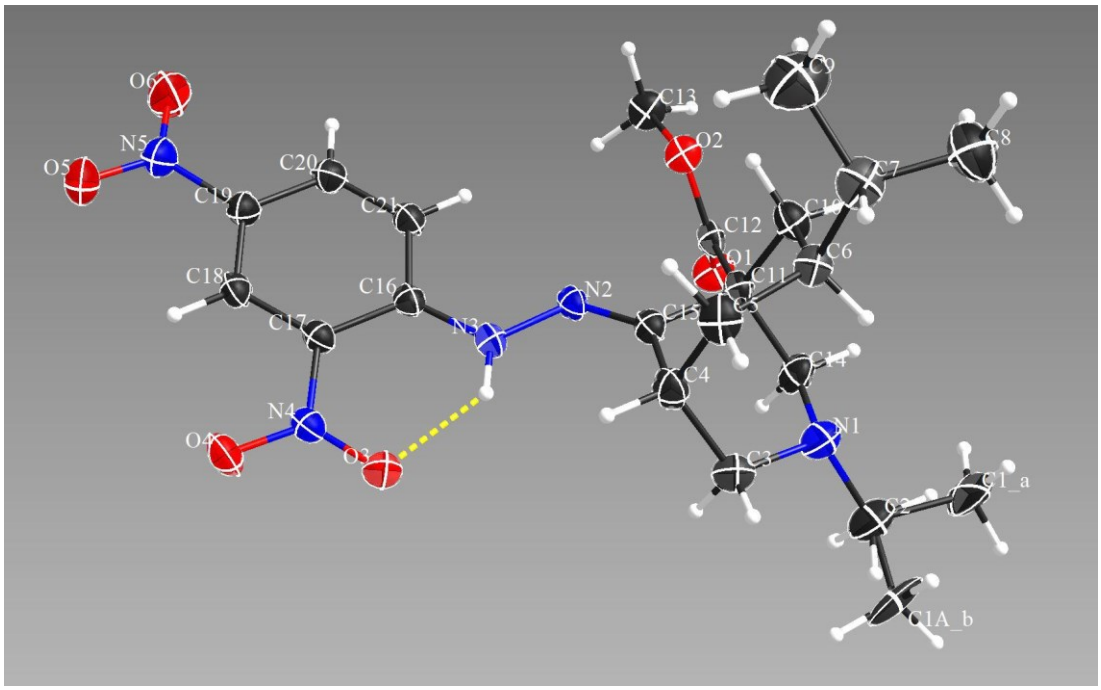

Table 9. Crystal data and structure refinement for s17phar6.

Identification code	s17phar6	
Empirical formula	C21 H29 N5 O6	
Formula weight	447.49	
Temperature	150.01(10) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	I2/a	
Unit cell dimensions	a = 7.74460(10) Å	α= 90°.
	b = 15.5385(2) Å	β= 91.337(2)°.
	c = 36.6455(7) Å	γ = 90°.
Volume	4408.70(12) Å^3	
Z	8	
Density (calculated)	1.348 Mg/m^3	
Absorption coefficient	0.834 mm^{-1}	
F(000)	1904	
Crystal size	0.200 x 0.100 x 0.040 mm^3	
Theta range for data collection	3.089 to 73.175°.	

Index ranges	-9<=h<=6, -19<=k<=19, -43<=l<=45
Reflections collected	25235
Independent reflections	4398 [R(int) = 0.0329]
Completeness to theta = 67.684°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.83146
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4398 / 0 / 308
Goodness-of-fit on F^2	1.076
Final R indices [I>2sigma(I)]	R1 = 0.0470, wR2 = 0.1337
R indices (all data)	R1 = 0.0509, wR2 = 0.1367
Extinction coefficient	n/a
Largest diff. peak and hole	0.371 and -0.433 e.$Å^{-3}$

Table 10. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for s17phar6. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	8355(2)	1648(1)	4224(1)	36(1)
N(2)	7050(2)	2879(1)	3272(1)	23(1)
N(3)	6019(2)	2440(1)	3019(1)	25(1)
N(4)	4058(2)	1516(1)	2456(1)	25(1)
N(5)	4068(2)	4106(1)	1718(1)	33(1)
O(1)	10746(2)	3600(1)	3613(1)	34(1)
O(2)	8413(1)	4448(1)	3617(1)	26(1)
O(3)	4434(2)	1125(1)	2741(1)	38(1)
O(4)	3170(2)	1188(1)	2213(1)	36(1)
O(5)	2996(2)	3753(1)	1516(1)	39(1)
O(6)	4661(2)	4824(1)	1663(1)	53(1)
C(1)	10464(6)	1291(2)	4724(1)	61(1)
C(1A)	8868(8)	205(5)	4506(2)	44(2)
C(2)	9572(3)	992(2)	4374(1)	49(1)
C(3)	7147(3)	1259(1)	3951(1)	35(1)
C(4)	5933(2)	1921(1)	3771(1)	29(1)
C(5)	4693(2)	2366(1)	4034(1)	32(1)
C(6)	5601(2)	2909(1)	4323(1)	26(1)
C(7)	4308(2)	3400(1)	4553(1)	35(1)

C(8)	5114(3)	3723(2)	4907(1)	48(1)
C(9)	3449(3)	4162(2)	4359(1)	58(1)
C(10)	6933(2)	3503(1)	4162(1)	28(1)
C(11)	8134(2)	3064(1)	3886(1)	23(1)
C(12)	9269(2)	3723(1)	3693(1)	24(1)
C(13)	9284(2)	5068(1)	3391(1)	30(1)
C(14)	9320(2)	2377(1)	4065(1)	32(1)
C(15)	7000(2)	2616(1)	3602(1)	23(1)
C(16)	5645(2)	2809(1)	2695(1)	22(1)
C(17)	4658(2)	2388(1)	2414(1)	22(1)
C(18)	4173(2)	2805(1)	2091(1)	25(1)
C(19)	4681(2)	3640(1)	2042(1)	26(1)
C(20)	5729(2)	4068(1)	2302(1)	28(1)
C(21)	6188(2)	3662(1)	2620(1)	25(1)

Table 11. Bond lengths [Å] for s17phar6.

N(1)-C(3)	1.482(2)
N(1)-C(14)	1.483(2)
N(1)-C(2)	1.487(2)
N(2)-C(15)	1.279(2)
N(2)-N(3)	1.3869(18)
N(3)-C(16)	1.347(2)
N(3)-H(3)	0.88(3)
N(4)-O(4)	1.2237(18)
N(4)-O(3)	1.2388(19)
N(4)-C(17)	1.443(2)
N(5)-O(6)	1.225(2)
N(5)-O(5)	1.229(2)
N(5)-C(19)	1.461(2)
O(1)-C(12)	1.203(2)
O(2)-C(12)	1.333(2)
O(2)-C(13)	1.448(2)
C(1)-C(2)	1.515(4)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800

C(1)-H(1C)	0.9800
C(1A)-C(2)	1.428(7)
C(1A)-H(1D)	0.9800
C(1A)-H(1E)	0.9800
C(1A)-H(1F)	0.9800
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(2)-H(2C)	0.9900
C(2)-H(2D)	0.9900
C(3)-C(4)	1.534(3)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(15)	1.501(2)
C(4)-C(5)	1.541(2)
C(4)-H(4)	1.0000
C(5)-C(6)	1.513(2)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-C(10)	1.514(2)
C(6)-C(7)	1.528(2)
C(6)-H(6)	1.0000
C(7)-C(8)	1.513(3)
C(7)-C(9)	1.526(3)
C(7)-H(7)	1.0000
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-C(11)	1.549(2)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(15)	1.515(2)
C(11)-C(12)	1.532(2)
C(11)-C(14)	1.545(2)
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800

C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(16)-C(21)	1.419(2)
C(16)-C(17)	1.427(2)
C(17)-C(18)	1.391(2)
C(18)-C(19)	1.369(2)
C(18)-H(18)	0.9500
C(19)-C(20)	1.402(2)
C(20)-C(21)	1.366(2)
C(20)-H(20)	0.9500
C(21)-H(21)	0.9500

Table 12. Bond angles [°] for s17phar6.

C(3)-N(1)-C(14)	111.35(14)
C(3)-N(1)-C(2)	110.79(16)
C(14)-N(1)-C(2)	110.39(16)
C(15)-N(2)-N(3)	116.39(14)
C(16)-N(3)-N(2)	119.21(14)
C(16)-N(3)-H(3)	115.1(16)
N(2)-N(3)-H(3)	125.6(16)
O(4)-N(4)-O(3)	121.87(14)
O(4)-N(4)-C(17)	119.39(14)
O(3)-N(4)-C(17)	118.73(13)
O(6)-N(5)-O(5)	123.89(16)
O(6)-N(5)-C(19)	117.92(15)
O(5)-N(5)-C(19)	118.19(15)
C(12)-O(2)-C(13)	116.43(13)
C(2)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
C(2)-C(1A)-H(1D)	109.5
C(2)-C(1A)-H(1E)	109.5

H(1D)-C(1A)-H(1E)	109.5
C(2)-C(1A)-H(1F)	109.5
H(1D)-C(1A)-H(1F)	109.5
H(1E)-C(1A)-H(1F)	109.5
C(1A)-C(2)-N(1)	118.0(3)
N(1)-C(2)-C(1)	112.1(2)
N(1)-C(2)-H(2A)	109.2
C(1)-C(2)-H(2A)	109.2
N(1)-C(2)-H(2B)	109.2
C(1)-C(2)-H(2B)	109.2
H(2A)-C(2)-H(2B)	107.9
C(1A)-C(2)-H(2C)	107.8
N(1)-C(2)-H(2C)	107.8
C(1A)-C(2)-H(2D)	107.8
N(1)-C(2)-H(2D)	107.8
H(2C)-C(2)-H(2D)	107.1
N(1)-C(3)-C(4)	112.82(15)
N(1)-C(3)-H(3A)	109.0
C(4)-C(3)-H(3A)	109.0
N(1)-C(3)-H(3B)	109.0
C(4)-C(3)-H(3B)	109.0
H(3A)-C(3)-H(3B)	107.8
C(15)-C(4)-C(3)	108.76(14)
C(15)-C(4)-C(5)	107.00(14)
C(3)-C(4)-C(5)	114.53(15)
C(15)-C(4)-H(4)	108.8
C(3)-C(4)-H(4)	108.8
C(5)-C(4)-H(4)	108.8
C(6)-C(5)-C(4)	113.72(14)
C(6)-C(5)-H(5A)	108.8
C(4)-C(5)-H(5A)	108.8
C(6)-C(5)-H(5B)	108.8
C(4)-C(5)-H(5B)	108.8
H(5A)-C(5)-H(5B)	107.7
C(5)-C(6)-C(10)	112.20(14)
C(5)-C(6)-C(7)	111.35(14)
C(10)-C(6)-C(7)	111.78(15)
C(5)-C(6)-H(6)	107.1
C(10)-C(6)-H(6)	107.1

C(7)-C(6)-H(6)	107.1
C(8)-C(7)-C(9)	107.92(19)
C(8)-C(7)-C(6)	112.10(16)
C(9)-C(7)-C(6)	114.61(16)
C(8)-C(7)-H(7)	107.3
C(9)-C(7)-H(7)	107.3
C(6)-C(7)-H(7)	107.3
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(6)-C(10)-C(11)	114.26(14)
C(6)-C(10)-H(10A)	108.7
C(11)-C(10)-H(10A)	108.7
C(6)-C(10)-H(10B)	108.7
C(11)-C(10)-H(10B)	108.7
H(10A)-C(10)-H(10B)	107.6
C(15)-C(11)-C(12)	108.72(13)
C(15)-C(11)-C(14)	107.64(13)
C(12)-C(11)-C(14)	108.42(13)
C(15)-C(11)-C(10)	107.69(12)
C(12)-C(11)-C(10)	111.54(13)
C(14)-C(11)-C(10)	112.68(14)
O(1)-C(12)-O(2)	123.71(16)
O(1)-C(12)-C(11)	124.41(15)
O(2)-C(12)-C(11)	111.86(13)
O(2)-C(13)-H(13A)	109.5
O(2)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
O(2)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5

H(13B)-C(13)-H(13C)	109.5
N(1)-C(14)-C(11)	113.22(14)
N(1)-C(14)-H(14A)	108.9
C(11)-C(14)-H(14A)	108.9
N(1)-C(14)-H(14B)	108.9
C(11)-C(14)-H(14B)	108.9
H(14A)-C(14)-H(14B)	107.7
N(2)-C(15)-C(4)	130.38(15)
N(2)-C(15)-C(11)	118.19(14)
C(4)-C(15)-C(11)	111.41(14)
N(3)-C(16)-C(21)	120.69(14)
N(3)-C(16)-C(17)	122.86(15)
C(21)-C(16)-C(17)	116.43(14)
C(18)-C(17)-C(16)	121.94(15)
C(18)-C(17)-N(4)	116.52(14)
C(16)-C(17)-N(4)	121.50(14)
C(19)-C(18)-C(17)	118.64(15)
C(19)-C(18)-H(18)	120.7
C(17)-C(18)-H(18)	120.7
C(18)-C(19)-C(20)	121.65(15)
C(18)-C(19)-N(5)	119.10(15)
C(20)-C(19)-N(5)	119.22(15)
C(21)-C(20)-C(19)	119.62(16)
C(21)-C(20)-H(20)	120.2
C(19)-C(20)-H(20)	120.2
C(20)-C(21)-C(16)	121.57(15)
C(20)-C(21)-H(21)	119.2
C(16)-C(21)-H(21)	119.2

Table 13. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for s17phar6. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	40(1)	30(1)	37(1)	4(1)	-5(1)	5(1)
N(2)	20(1)	25(1)	24(1)	-4(1)	-3(1)	1(1)

N(3)	28(1)	24(1)	24(1)	-2(1)	-5(1)	-2(1)
N(4)	25(1)	23(1)	26(1)	-5(1)	1(1)	0(1)
N(5)	41(1)	33(1)	26(1)	1(1)	-3(1)	5(1)
O(1)	20(1)	41(1)	43(1)	2(1)	4(1)	2(1)
O(2)	19(1)	29(1)	31(1)	1(1)	2(1)	-2(1)
O(3)	51(1)	24(1)	37(1)	4(1)	-13(1)	-6(1)
O(4)	44(1)	33(1)	30(1)	-8(1)	-5(1)	-12(1)
O(5)	43(1)	45(1)	29(1)	-1(1)	-10(1)	4(1)
O(6)	82(1)	35(1)	41(1)	12(1)	-14(1)	-9(1)
C(1)	83(3)	40(2)	58(2)	13(2)	-43(2)	11(2)
C(1A)	37(3)	48(4)	47(4)	38(3)	13(3)	13(3)
C(2)	60(1)	39(1)	48(1)	7(1)	-12(1)	13(1)
C(3)	43(1)	26(1)	36(1)	1(1)	-2(1)	-1(1)
C(4)	32(1)	30(1)	27(1)	-1(1)	-3(1)	-7(1)
C(5)	25(1)	40(1)	32(1)	1(1)	2(1)	-7(1)
C(6)	22(1)	31(1)	25(1)	1(1)	2(1)	1(1)
C(7)	28(1)	42(1)	35(1)	2(1)	9(1)	0(1)
C(8)	47(1)	58(1)	40(1)	-8(1)	10(1)	2(1)
C(9)	46(1)	64(2)	63(2)	6(1)	12(1)	11(1)
C(10)	29(1)	31(1)	24(1)	-5(1)	4(1)	-3(1)
C(11)	20(1)	27(1)	22(1)	-2(1)	-2(1)	0(1)
C(12)	20(1)	30(1)	20(1)	-5(1)	-4(1)	-1(1)
C(13)	24(1)	32(1)	34(1)	3(1)	3(1)	-5(1)
C(14)	27(1)	36(1)	31(1)	3(1)	-7(1)	3(1)
C(15)	20(1)	26(1)	24(1)	-4(1)	-2(1)	2(1)
C(16)	20(1)	24(1)	23(1)	-4(1)	0(1)	2(1)
C(17)	22(1)	22(1)	24(1)	-4(1)	1(1)	1(1)
C(18)	24(1)	28(1)	22(1)	-6(1)	-1(1)	2(1)
C(19)	29(1)	27(1)	22(1)	0(1)	0(1)	4(1)
C(20)	32(1)	22(1)	29(1)	-2(1)	1(1)	-1(1)
C(21)	25(1)	24(1)	26(1)	-5(1)	-2(1)	-1(1)

Table 14. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{3}) for s17phar6.

	x	y	z	U(eq)

H(3)	5630(30)	1909(17)	3045(7)	42(6)
H(1A)	11209	1784	4672	92
H(1B)	11166	822	4827	92
H(1C)	9595	1463	4900	92
H(1D)	8382	-128	4301	65
H(1E)	7957	332	4680	65
H(1F)	9783	-131	4629	65
H(2A)	10454	862	4191	59
H(2B)	8930	454	4423	59
H(2C)	10398	847	4182	59
H(2D)	10244	1261	4577	59
H(3A)	6448	814	4072	42
H(3B)	7821	971	3760	42
H(4)	5236	1629	3573	35
H(5A)	3888	2737	3891	39
H(5B)	3998	1921	4156	39
H(6)	6235	2504	4491	31
H(7)	3373	2987	4617	42
H(8A)	4216	3970	5059	72
H(8B)	5978	4164	4854	72
H(8C)	5672	3243	5037	72
H(9A)	2524	4389	4510	87
H(9B)	2962	3975	4123	87
H(9C)	4308	4614	4320	87
H(10A)	7652	3747	4364	34
H(10B)	6327	3987	4038	34
H(13A)	8541	5572	3353	45
H(13B)	9532	4805	3155	45
H(13C)	10368	5245	3512	45
H(14A)	10112	2152	3880	38
H(14B)	10032	2653	4260	38
H(18)	3502	2516	1909	30
H(20)	6118	4637	2256	33
H(21)	6888	3958	2796	31

Table 15. Torsion angles [°] for s17phar6.

C(15)-N(2)-N(3)-C(16)	162.34(14)
C(3)-N(1)-C(2)-C(1A)	-50.3(4)
C(14)-N(1)-C(2)-C(1A)	-174.1(4)
C(3)-N(1)-C(2)-C(1)	-163.5(3)
C(14)-N(1)-C(2)-C(1)	72.7(3)
C(14)-N(1)-C(3)-C(4)	-53.3(2)
C(2)-N(1)-C(3)-C(4)	-176.58(17)
N(1)-C(3)-C(4)-C(15)	56.1(2)
N(1)-C(3)-C(4)-C(5)	-63.5(2)
C(15)-C(4)-C(5)-C(6)	-56.58(19)
C(3)-C(4)-C(5)-C(6)	64.0(2)
C(4)-C(5)-C(6)-C(10)	48.5(2)
C(4)-C(5)-C(6)-C(7)	174.62(15)
C(5)-C(6)-C(7)-C(8)	162.58(17)
C(10)-C(6)-C(7)-C(8)	-71.0(2)
C(5)-C(6)-C(7)-C(9)	-74.0(2)
C(10)-C(6)-C(7)-C(9)	52.4(2)
C(5)-C(6)-C(10)-C(11)	-46.5(2)
C(7)-C(6)-C(10)-C(11)	-172.39(14)
C(6)-C(10)-C(11)-C(15)	52.54(18)
C(6)-C(10)-C(11)-C(12)	171.75(13)
C(6)-C(10)-C(11)-C(14)	-66.03(18)
C(13)-O(2)-C(12)-O(1)	7.1(2)
C(13)-O(2)-C(12)-C(11)	-171.70(13)
C(15)-C(11)-C(12)-O(1)	-98.61(18)
C(14)-C(11)-C(12)-O(1)	18.1(2)
C(10)-C(11)-C(12)-O(1)	142.78(16)
C(15)-C(11)-C(12)-O(2)	80.15(16)
C(14)-C(11)-C(12)-O(2)	-163.10(13)
C(10)-C(11)-C(12)-O(2)	-38.46(17)
C(3)-N(1)-C(14)-C(11)	53.6(2)
C(2)-N(1)-C(14)-C(11)	177.10(16)
C(15)-C(11)-C(14)-N(1)	-55.82(19)
C(12)-C(11)-C(14)-N(1)	-173.27(14)
C(10)-C(11)-C(14)-N(1)	62.77(19)
N(3)-N(2)-C(15)-C(4)	-3.2(2)
N(3)-N(2)-C(15)-C(11)	178.75(13)
C(3)-C(4)-C(15)-N(2)	122.05(19)

C(5)-C(4)-C(15)-N(2)	-113.73(19)
C(3)-C(4)-C(15)-C(11)	-59.75(18)
C(5)-C(4)-C(15)-C(11)	64.46(17)
C(12)-C(11)-C(15)-N(2)	-5.14(19)
C(14)-C(11)-C(15)-N(2)	-122.39(16)
C(10)-C(11)-C(15)-N(2)	115.86(16)
C(12)-C(11)-C(15)-C(4)	176.42(13)
C(14)-C(11)-C(15)-C(4)	59.17(17)
C(10)-C(11)-C(15)-C(4)	-62.58(17)
N(2)-N(3)-C(16)-C(21)	-4.6(2)
N(2)-N(3)-C(16)-C(17)	177.20(13)
N(3)-C(16)-C(17)-C(18)	174.93(15)
C(21)-C(16)-C(17)-C(18)	-3.4(2)
N(3)-C(16)-C(17)-N(4)	-2.7(2)
C(21)-C(16)-C(17)-N(4)	178.98(14)
O(4)-N(4)-C(17)-C(18)	-0.1(2)
O(3)-N(4)-C(17)-C(18)	-178.73(15)
O(4)-N(4)-C(17)-C(16)	177.72(14)
O(3)-N(4)-C(17)-C(16)	-0.9(2)
C(16)-C(17)-C(18)-C(19)	0.9(2)
N(4)-C(17)-C(18)-C(19)	178.64(14)
C(17)-C(18)-C(19)-C(20)	2.6(2)
C(17)-C(18)-C(19)-N(5)	-175.32(14)
O(6)-N(5)-C(19)-C(18)	-173.54(17)
O(5)-N(5)-C(19)-C(18)	6.2(2)
O(6)-N(5)-C(19)-C(20)	8.5(3)
O(5)-N(5)-C(19)-C(20)	-171.81(16)
C(18)-C(19)-C(20)-C(21)	-3.4(3)
N(5)-C(19)-C(20)-C(21)	174.49(15)
C(19)-C(20)-C(21)-C(16)	0.7(3)
N(3)-C(16)-C(21)-C(20)	-175.80(15)
C(17)-C(16)-C(21)-C(20)	2.5(2)

Table 16. Hydrogen bonds for s17phar6 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

N(3)-H(3)...O(3)	0.88(3)	1.88(3)	2.5809(19)	135(2)

s18phar4: methyl (1*R*,5*R*,7*S*,*E*)-9-(2-(2,4-dinitrophenyl)hydrazinylidene)-3-ethyl-7-methyl-3-azabicyclo [3.3.1]nonane-1-carboxylate (**17a**) and methyl (1*S*,5*S*,7*R*,*E*)-9-(2-(2,4-dinitrophenyl) hydrazinylidene)-3-ethyl-7-methyl-3-azabicyclo[3.3.1]nonane-1-carboxylate (twin-packed) (**17b**)

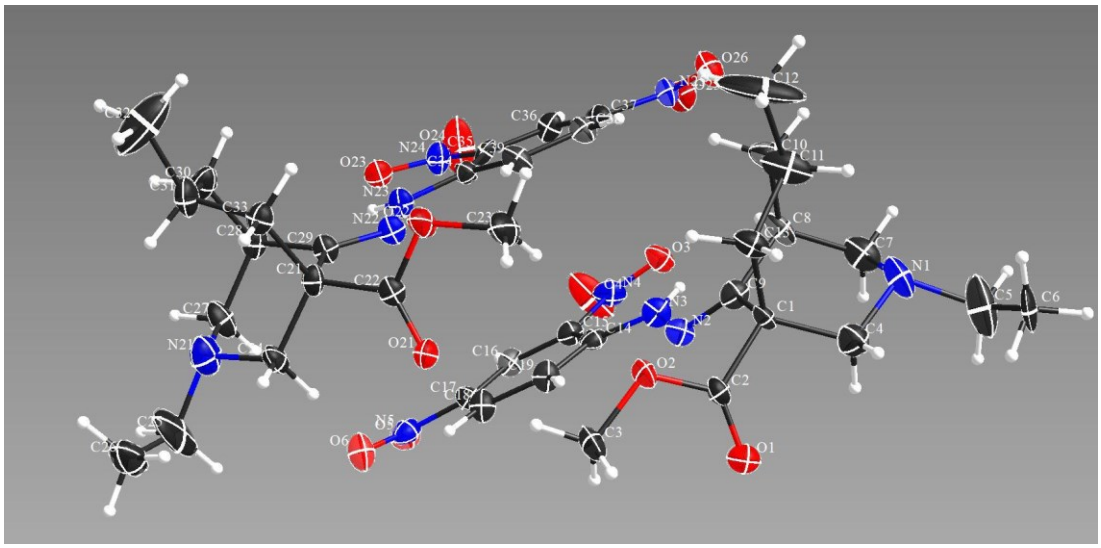

Table 17. Crystal data and structure refinement for s18phar4.

Identification code	s18phar4	
Empirical formula	C18.60 H23.80 N5 O6	
Formula weight	413.42	
Temperature	149.9(4) K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.7392(4) Å	α= 110.066(11)°.
	b = 15.8949(16) Å	β= 90.729(7)°.
	c = 17.396(2) Å	γ = 90.190(7)°.
Volume	2009.8(4) Å^3	
Z	4	
Density (calculated)	1.366 Mg/m^3	

Absorption coefficient	0.871 mm^{-1}
F(000)	874
Crystal size	0.425 x 0.039 x 0.025 mm^3
Theta range for data collection	2.705 to 69.746°.
Index ranges	-9<=h<=9, -18<=k<=19, -20<=l<=20
Reflections collected	11165
Independent reflections	11165 [R(int) = ?]
Completeness to theta = 67.684°	100.0 %
Absorption correction	Gaussian
Max. and min. transmission	0.981 and 0.838
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11165 / 2 / 556
Goodness-of-fit on F^2	0.786
Final R indices [I>2sigma(I)]	R1 = 0.0621, wR2 = 0.1311
R indices (all data)	R1 = 0.1407, wR2 = 0.1536
Extinction coefficient	n/a
Largest diff. peak and hole	0.714 and -0.310 e.$Å^{-3}$

Table 18. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for s18phar4. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	8716(7)	-2209(4)	2152(3)	37(1)
N(2)	7692(6)	436(3)	2834(3)	22(1)
N(3)	6893(7)	875(4)	3579(3)	24(1)
N(4)	5601(6)	1934(4)	5204(3)	30(1)
N(5)	6818(6)	4625(4)	4545(3)	29(1)
O(1)	11027(5)	-124(3)	1544(3)	32(1)
O(2)	8520(5)	319(3)	1164(3)	30(1)
O(3)	5372(5)	1116(3)	4986(2)	30(1)
O(4)	5265(8)	2441(3)	5894(3)	63(2)
O(5)	6752(5)	5046(3)	5284(2)	30(1)
O(6)	6930(6)	4943(3)	4005(3)	37(1)
C(1)	8380(6)	-871(4)	1713(3)	17(1)
C(2)	9475(6)	-197(4)	1475(3)	19(1)
C(3)	9449(8)	1036(4)	995(4)	38(2)

C(4)	9607(7)	-1582(4)	1835(4)	32(2)
C(5)	10037(12)	-2838(5)	2319(5)	61(3)
C(6)	10556(15)	-3449(7)	1573(6)	37(3)
C(7)	7767(9)	-1740(5)	2902(4)	34(2)
C(8)	6491(7)	-1061(4)	2788(3)	27(1)
C(9)	7493(7)	-404(4)	2515(3)	24(1)
C(10)	5068(8)	-1480(5)	2135(3)	32(2)
C(11)	5710(9)	-1863(5)	1284(4)	40(2)
C(12)	4191(10)	-2125(6)	661(4)	83(4)
C(13)	6949(7)	-1276(4)	1066(3)	25(1)
C(14)	6796(6)	1777(4)	3830(3)	20(1)
C(15)	6249(7)	2327(4)	4606(3)	22(1)
C(16)	6240(7)	3250(4)	4849(3)	24(1)
C(17)	6755(7)	3641(4)	4296(3)	23(1)
C(18)	7229(8)	3137(4)	3503(3)	26(2)
C(19)	7260(7)	2213(4)	3280(3)	26(1)
N(21)	3832(7)	5092(4)	2137(3)	37(1)
N(22)	2714(6)	2967(4)	2868(3)	22(1)
N(23)	1904(6)	3097(4)	3606(3)	21(1)
N(24)	574(6)	3213(4)	5214(3)	28(1)
N(25)	1805(6)	58(4)	4551(3)	25(1)
O(21)	6052(4)	2547(3)	1596(2)	24(1)
O(22)	3523(4)	1828(3)	1211(2)	26(1)
O(23)	371(5)	3879(3)	5002(2)	28(1)
O(24)	198(8)	3222(4)	5905(3)	63(2)
O(25)	1746(5)	160(3)	5286(2)	31(1)
O(26)	1940(6)	-688(3)	4008(3)	36(1)
C(21)	3456(7)	3426(4)	1742(3)	20(1)
C(22)	4510(6)	2567(4)	1511(3)	20(1)
C(23)	4445(7)	998(4)	1063(4)	37(2)
C(24)	4696(7)	4209(4)	1834(3)	24(1)
C(25)	5127(12)	5828(5)	2240(6)	71(3)
C(26)	5484(15)	5848(9)	1353(8)	48(4)
C(27)	2921(9)	5221(4)	2912(4)	32(2)
C(28)	1622(7)	4452(4)	2833(3)	26(1)
C(29)	2593(7)	3588(4)	2555(3)	20(1)
C(30)	177(7)	4362(5)	2189(4)	28(2)
C(31)	755(8)	4100(5)	1326(4)	32(2)
C(32)	-766(9)	3871(6)	729(4)	72(3)

C(33)	1990(7)	3337(4)	1097(3)	23(1)
C(34)	1797(6)	2359(4)	3842(3)	20(1)
C(35)	1214(6)	2392(4)	4619(3)	19(1)
C(36)	1212(7)	1641(4)	4856(3)	25(1)
C(37)	1733(6)	839(4)	4307(3)	22(1)
C(38)	2201(7)	767(4)	3513(3)	22(1)
C(39)	2264(7)	1508(4)	3287(3)	25(1)

Table 19. Bond lengths [Å] for s18phar4.

N(1)-C(4)	1.469(7)
N(1)-C(7)	1.469(8)
N(1)-C(5)	1.526(9)
N(2)-C(9)	1.265(8)
N(2)-N(3)	1.396(6)
N(3)-C(14)	1.351(8)
N(3)-H(3)	0.83(2)
N(4)-O(4)	1.227(6)
N(4)-O(3)	1.234(7)
N(4)-C(15)	1.476(8)
N(5)-O(6)	1.213(7)
N(5)-O(5)	1.231(6)
N(5)-C(17)	1.473(8)
O(1)-C(2)	1.207(6)
O(2)-C(2)	1.344(6)
O(2)-C(3)	1.461(7)
C(1)-C(9)	1.512(7)
C(1)-C(2)	1.531(7)
C(1)-C(13)	1.541(7)
C(1)-C(4)	1.546(7)
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(6)	1.393(12)

C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(7)-C(8)	1.526(9)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.503(8)
C(8)-C(10)	1.546(8)
C(8)-H(8)	1.0000
C(10)-C(11)	1.487(8)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(13)	1.476(8)
C(11)-C(12)	1.543(9)
C(11)-H(11)	1.0000
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(15)	1.405(7)
C(14)-C(19)	1.410(8)
C(15)-C(16)	1.381(8)
C(16)-C(17)	1.373(8)
C(16)-H(16)	0.9500
C(17)-C(18)	1.391(7)
C(18)-C(19)	1.385(8)
C(18)-H(18)	0.9500
C(19)-H(19)	0.9500
N(21)-C(27)	1.480(7)
N(21)-C(24)	1.483(7)
N(21)-C(25)	1.501(9)
N(22)-C(29)	1.283(8)
N(22)-N(23)	1.387(6)
N(23)-C(34)	1.371(8)
N(23)-H(23)	0.84(2)
N(24)-O(24)	1.236(6)

N(24)-O(23)	1.244(6)
N(24)-C(35)	1.452(7)
N(25)-O(25)	1.233(6)
N(25)-O(26)	1.242(7)
N(25)-C(37)	1.445(8)
O(21)-C(22)	1.202(6)
O(22)-C(22)	1.342(6)
O(22)-C(23)	1.447(7)
C(21)-C(29)	1.513(7)
C(21)-C(22)	1.527(7)
C(21)-C(24)	1.532(7)
C(21)-C(33)	1.557(7)
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-C(26)	1.580(14)
C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-C(28)	1.549(8)
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(28)-C(29)	1.498(8)
C(28)-C(30)	1.543(8)
C(28)-H(28)	1.0000
C(30)-C(31)	1.489(8)
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900
C(31)-C(33)	1.493(8)
C(31)-C(32)	1.518(9)
C(31)-H(31)	1.0000
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-H(33A)	0.9900

C(33)-H(33B)	0.9900
C(34)-C(35)	1.416(7)
C(34)-C(39)	1.418(8)
C(35)-C(36)	1.389(8)
C(36)-C(37)	1.369(8)
C(36)-H(36)	0.9500
C(37)-C(38)	1.398(7)
C(38)-C(39)	1.365(8)
C(38)-H(38)	0.9500
C(39)-H(39)	0.9500

Table 20. Bond angles [°] for s18phar4.

C(4)-N(1)-C(7)	111.9(5)
C(4)-N(1)-C(5)	109.2(6)
C(7)-N(1)-C(5)	109.9(5)
C(9)-N(2)-N(3)	118.1(5)
C(14)-N(3)-N(2)	117.7(5)
C(14)-N(3)-H(3)	117(5)
N(2)-N(3)-H(3)	126(5)
O(4)-N(4)-O(3)	122.5(6)
O(4)-N(4)-C(15)	118.3(6)
O(3)-N(4)-C(15)	119.2(5)
O(6)-N(5)-O(5)	126.2(6)
O(6)-N(5)-C(17)	117.3(5)
O(5)-N(5)-C(17)	116.6(6)
C(2)-O(2)-C(3)	116.0(4)
C(9)-C(1)-C(2)	110.0(5)
C(9)-C(1)-C(13)	107.1(4)
C(2)-C(1)-C(13)	110.5(4)
C(9)-C(1)-C(4)	108.2(5)
C(2)-C(1)-C(4)	107.9(4)
C(13)-C(1)-C(4)	113.2(5)
O(1)-C(2)-O(2)	122.1(5)
O(1)-C(2)-C(1)	125.2(5)
O(2)-C(2)-C(1)	112.7(4)

O(2)-C(3)-H(3A)	109.5
O(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
O(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
N(1)-C(4)-C(1)	112.5(5)
N(1)-C(4)-H(4A)	109.1
C(1)-C(4)-H(4A)	109.1
N(1)-C(4)-H(4B)	109.1
C(1)-C(4)-H(4B)	109.1
H(4A)-C(4)-H(4B)	107.8
C(6)-C(5)-N(1)	108.5(7)
C(6)-C(5)-H(5A)	110.0
N(1)-C(5)-H(5A)	110.0
C(6)-C(5)-H(5B)	110.0
N(1)-C(5)-H(5B)	110.0
H(5A)-C(5)-H(5B)	108.4
C(5)-C(6)-H(6A)	109.5
C(5)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(5)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
N(1)-C(7)-C(8)	112.5(5)
N(1)-C(7)-H(7A)	109.1
C(8)-C(7)-H(7A)	109.1
N(1)-C(7)-H(7B)	109.1
C(8)-C(7)-H(7B)	109.1
H(7A)-C(7)-H(7B)	107.8
C(9)-C(8)-C(7)	107.7(5)
C(9)-C(8)-C(10)	107.6(5)
C(7)-C(8)-C(10)	113.9(5)
C(9)-C(8)-H(8)	109.2
C(7)-C(8)-H(8)	109.2
C(10)-C(8)-H(8)	109.2
N(2)-C(9)-C(8)	131.5(5)
N(2)-C(9)-C(1)	117.5(5)
C(8)-C(9)-C(1)	111.0(5)

C(11)-C(10)-C(8)	114.4(5)
C(11)-C(10)-H(10A)	108.7
C(8)-C(10)-H(10A)	108.7
C(11)-C(10)-H(10B)	108.7
C(8)-C(10)-H(10B)	108.7
H(10A)-C(10)-H(10B)	107.6
C(13)-C(11)-C(10)	113.8(6)
C(13)-C(11)-C(12)	110.6(6)
C(10)-C(11)-C(12)	110.9(6)
C(13)-C(11)-H(11)	107.1
C(10)-C(11)-H(11)	107.1
C(12)-C(11)-H(11)	107.1
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(11)-C(13)-C(1)	114.5(5)
C(11)-C(13)-H(13A)	108.6
C(1)-C(13)-H(13A)	108.6
C(11)-C(13)-H(13B)	108.6
C(1)-C(13)-H(13B)	108.6
H(13A)-C(13)-H(13B)	107.6
N(3)-C(14)-C(15)	124.9(6)
N(3)-C(14)-C(19)	118.6(5)
C(15)-C(14)-C(19)	116.5(6)
C(16)-C(15)-C(14)	122.9(6)
C(16)-C(15)-N(4)	116.3(5)
C(14)-C(15)-N(4)	120.8(6)
C(17)-C(16)-C(15)	118.1(5)
C(17)-C(16)-H(16)	121.0
C(15)-C(16)-H(16)	121.0
C(16)-C(17)-C(18)	122.1(6)
C(16)-C(17)-N(5)	119.5(5)
C(18)-C(17)-N(5)	118.4(6)
C(19)-C(18)-C(17)	118.6(6)
C(19)-C(18)-H(18)	120.7
C(17)-C(18)-H(18)	120.7

C(18)-C(19)-C(14)	121.6(5)
C(18)-C(19)-H(19)	119.2
C(14)-C(19)-H(19)	119.2
C(27)-N(21)-C(24)	111.5(5)
C(27)-N(21)-C(25)	110.9(6)
C(24)-N(21)-C(25)	110.0(5)
C(29)-N(22)-N(23)	117.9(5)
C(34)-N(23)-N(22)	115.8(5)
C(34)-N(23)-H(23)	119(4)
N(22)-N(23)-H(23)	124(5)
O(24)-N(24)-O(23)	122.0(5)
O(24)-N(24)-C(35)	119.2(6)
O(23)-N(24)-C(35)	118.7(5)
O(25)-N(25)-O(26)	123.0(6)
O(25)-N(25)-C(37)	118.8(5)
O(26)-N(25)-C(37)	118.3(5)
C(22)-O(22)-C(23)	114.4(4)
C(29)-C(21)-C(22)	110.0(5)
C(29)-C(21)-C(24)	108.3(5)
C(22)-C(21)-C(24)	108.2(4)
C(29)-C(21)-C(33)	106.9(4)
C(22)-C(21)-C(33)	110.3(4)
C(24)-C(21)-C(33)	113.1(5)
O(21)-C(22)-O(22)	123.2(5)
O(21)-C(22)-C(21)	124.2(5)
O(22)-C(22)-C(21)	112.6(4)
O(22)-C(23)-H(23A)	109.5
O(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
O(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
N(21)-C(24)-C(21)	112.7(5)
N(21)-C(24)-H(24A)	109.0
C(21)-C(24)-H(24A)	109.0
N(21)-C(24)-H(24B)	109.0
C(21)-C(24)-H(24B)	109.0
H(24A)-C(24)-H(24B)	107.8
N(21)-C(25)-C(26)	106.5(8)

N(21)-C(25)-H(25A)	110.4
C(26)-C(25)-H(25A)	110.4
N(21)-C(25)-H(25B)	110.4
C(26)-C(25)-H(25B)	110.4
H(25A)-C(25)-H(25B)	108.6
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
N(21)-C(27)-C(28)	112.0(5)
N(21)-C(27)-H(27A)	109.2
C(28)-C(27)-H(27A)	109.2
N(21)-C(27)-H(27B)	109.2
C(28)-C(27)-H(27B)	109.2
H(27A)-C(27)-H(27B)	107.9
C(29)-C(28)-C(30)	106.5(5)
C(29)-C(28)-C(27)	108.0(5)
C(30)-C(28)-C(27)	113.6(5)
C(29)-C(28)-H(28)	109.6
C(30)-C(28)-H(28)	109.6
C(27)-C(28)-H(28)	109.6
N(22)-C(29)-C(28)	130.7(5)
N(22)-C(29)-C(21)	117.1(5)
C(28)-C(29)-C(21)	112.0(5)
C(31)-C(30)-C(28)	115.5(5)
C(31)-C(30)-H(30A)	108.4
C(28)-C(30)-H(30A)	108.4
C(31)-C(30)-H(30B)	108.4
C(28)-C(30)-H(30B)	108.4
H(30A)-C(30)-H(30B)	107.5
C(30)-C(31)-C(33)	113.1(5)
C(30)-C(31)-C(32)	111.5(6)
C(33)-C(31)-C(32)	109.3(6)
C(30)-C(31)-H(31)	107.5
C(33)-C(31)-H(31)	107.5
C(32)-C(31)-H(31)	107.5
C(31)-C(32)-H(32A)	109.5

C(31)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(31)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(31)-C(33)-C(21)	114.1(5)
C(31)-C(33)-H(33A)	108.7
C(21)-C(33)-H(33A)	108.7
C(31)-C(33)-H(33B)	108.7
C(21)-C(33)-H(33B)	108.7
H(33A)-C(33)-H(33B)	107.6
N(23)-C(34)-C(35)	123.4(5)
N(23)-C(34)-C(39)	119.6(5)
C(35)-C(34)-C(39)	116.9(6)
C(36)-C(35)-C(34)	122.0(5)
C(36)-C(35)-N(24)	116.2(5)
C(34)-C(35)-N(24)	121.8(6)
C(37)-C(36)-C(35)	118.8(5)
C(37)-C(36)-H(36)	120.6
C(35)-C(36)-H(36)	120.6
C(36)-C(37)-C(38)	120.8(6)
C(36)-C(37)-N(25)	119.7(5)
C(38)-C(37)-N(25)	119.4(6)
C(39)-C(38)-C(37)	120.5(6)
C(39)-C(38)-H(38)	119.7
C(37)-C(38)-H(38)	119.7
C(38)-C(39)-C(34)	120.7(5)
C(38)-C(39)-H(39)	119.7
C(34)-C(39)-H(39)	119.7

Table 21. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for s18phar4. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	58(3)	21(3)	36(3)	14(2)	-1(3)	-4(3)

N(2)	27(2)	20(3)	16(2)	-1(2)	4(2)	0(2)
N(3)	31(3)	27(4)	10(2)	2(2)	4(2)	1(2)
N(4)	27(3)	37(4)	24(3)	6(2)	7(2)	-3(3)
N(5)	24(3)	28(4)	29(3)	2(3)	-5(2)	1(2)
O(1)	27(2)	31(3)	41(3)	15(2)	-2(2)	-4(2)
O(2)	26(2)	25(3)	47(3)	24(2)	7(2)	2(2)
O(3)	33(2)	26(3)	30(2)	7(2)	8(2)	-4(2)
O(4)	114(5)	39(4)	26(3)	-5(2)	41(3)	-14(3)
O(5)	29(2)	25(3)	26(2)	-3(2)	0(2)	0(2)
O(6)	51(3)	30(3)	33(2)	14(2)	-2(2)	4(2)
C(1)	21(2)	13(3)	19(3)	7(2)	3(2)	-3(2)
C(2)	26(3)	13(3)	16(3)	3(2)	2(2)	-1(2)
C(3)	40(3)	24(4)	60(4)	26(3)	8(3)	0(3)
C(4)	32(3)	31(4)	35(3)	14(3)	0(3)	-2(3)
C(5)	112(7)	30(5)	46(4)	20(4)	6(5)	15(5)
C(6)	57(7)	11(5)	43(6)	8(5)	7(5)	15(5)
C(7)	48(4)	32(5)	21(3)	7(3)	0(3)	-10(3)
C(8)	42(3)	17(3)	17(3)	2(2)	7(2)	-6(3)
C(9)	25(3)	25(4)	19(3)	3(3)	2(2)	2(3)
C(10)	33(3)	31(4)	24(3)	1(3)	4(3)	-10(3)
C(11)	47(4)	48(5)	20(3)	4(3)	5(3)	-20(4)
C(12)	76(5)	116(8)	29(4)	-11(4)	6(4)	-78(6)
C(13)	29(3)	24(4)	19(3)	4(2)	3(2)	-9(2)
C(14)	16(2)	20(4)	18(3)	0(2)	-3(2)	-2(2)
C(15)	21(3)	23(4)	17(3)	3(3)	3(2)	2(3)
C(16)	28(3)	21(4)	17(3)	-2(3)	0(2)	3(3)
C(17)	26(3)	18(4)	21(3)	1(2)	-3(2)	-3(2)
C(18)	34(3)	25(4)	19(3)	6(3)	-1(2)	4(3)
C(19)	32(3)	25(4)	18(3)	5(2)	1(2)	4(3)
N(21)	45(3)	26(3)	36(3)	7(3)	11(2)	10(3)
N(22)	26(2)	24(3)	15(2)	6(2)	7(2)	2(2)
N(23)	28(2)	24(3)	14(2)	8(2)	7(2)	3(2)
N(24)	35(3)	27(4)	22(3)	10(2)	10(2)	11(2)
N(25)	30(3)	21(3)	25(3)	11(2)	0(2)	0(2)
O(21)	23(2)	21(2)	30(2)	9(2)	2(2)	4(2)
O(22)	25(2)	15(2)	34(2)	2(2)	6(2)	2(2)
O(23)	27(2)	30(3)	27(2)	9(2)	7(2)	3(2)
O(24)	111(4)	58(4)	26(3)	21(2)	43(3)	41(3)
O(25)	35(2)	39(3)	24(2)	17(2)	0(2)	1(2)

O(26)	51(3)	22(3)	35(2)	10(2)	-4(2)	-4(2)
C(21)	26(3)	18(3)	17(3)	5(2)	4(2)	6(2)
C(22)	25(3)	19(3)	15(3)	5(2)	6(2)	2(2)
C(23)	33(3)	16(4)	54(4)	2(3)	4(3)	2(3)
C(24)	28(3)	14(3)	30(3)	7(2)	8(2)	1(2)
C(25)	85(6)	14(4)	113(8)	18(5)	41(6)	7(4)
C(26)	39(6)	38(8)	73(9)	27(7)	23(6)	6(6)
C(27)	49(4)	15(4)	28(3)	2(3)	8(3)	2(3)
C(28)	30(3)	26(4)	21(3)	7(2)	8(2)	10(3)
C(29)	26(3)	20(3)	14(3)	5(2)	5(2)	2(2)
C(30)	22(3)	37(4)	30(3)	16(3)	6(2)	10(3)
C(31)	39(3)	24(4)	36(4)	15(3)	5(3)	11(3)
C(32)	54(4)	114(8)	35(4)	9(5)	-6(4)	41(5)
C(33)	26(3)	26(4)	19(3)	9(2)	1(2)	3(2)
C(34)	20(2)	21(4)	21(3)	9(2)	0(2)	-2(2)
C(35)	16(2)	26(4)	16(3)	6(3)	2(2)	9(2)
C(36)	27(3)	32(4)	16(3)	11(3)	3(2)	6(3)
C(37)	20(2)	27(4)	20(3)	12(3)	-2(2)	-3(2)
C(38)	28(3)	19(4)	15(3)	1(2)	-3(2)	-3(3)
C(39)	33(3)	24(4)	15(3)	4(2)	0(2)	-8(3)

Table 22. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for s18phar4.

	x	y	z	U(eq)
H(3)	6500(70)	630(40)	3890(30)	34(19)
H(3A)	10226	777	535	57
H(3B)	10125	1385	1481	57
H(3C)	8619	1428	857	57
H(4A)	10136	-1922	1304	38
H(4B)	10550	-1276	2221	38
H(5A)	11048	-2491	2622	73
H(5B)	9516	-3159	2658	73
H(6A)	9539	-3677	1220	56

H(6B)	11154	-3949	1667	56
H(6C)	11340	-3152	1307	56
H(7A)	8602	-1426	3344	41
H(7B)	7130	-2185	3074	41
H(8)	5937	-735	3323	32
H(10A)	4472	-1959	2274	38
H(10B)	4204	-1014	2157	38
H(11)	6333	-2427	1241	49
H(12A)	4632	-2256	107	124
H(12B)	3372	-1629	784	124
H(12C)	3605	-2658	697	124
H(13A)	6304	-781	974	30
H(13B)	7499	-1625	543	30
H(16)	5887	3605	5382	29
H(18)	7525	3421	3123	32
H(19)	7603	1864	2743	31
H(23)	1620(70)	3600(20)	3940(30)	35(19)
H(23A)	3619	497	913	55
H(23B)	5083	1021	1560	55
H(23C)	5257	914	616	55
H(24A)	5643	4200	2219	29
H(24B)	5216	4130	1297	29
H(25A)	6208	5709	2493	85
H(25B)	4662	6410	2593	85
H(26A)	5888	5259	1003	72
H(26B)	6370	6302	1387	72
H(26C)	4416	5995	1121	72
H(27A)	2295	5797	3075	38
H(27B)	3781	5255	3348	38
H(28)	1097	4541	3377	31
H(30A)	-672	3911	2226	34
H(30B)	-428	4942	2331	34
H(31)	1367	4628	1265	38
H(32A)	-379	3852	189	108
H(32B)	-1659	4328	924	108
H(32C)	-1242	3285	688	108
H(33A)	2520	3288	569	28
H(33B)	1338	2776	1016	28
H(36)	856	1683	5388	30

H(38)	2477	197	3129	27
H(39)	2626	1452	2752	29

Table 23. Torsion angles [°] for s18phar4.

C(9)-N(2)-N(3)-C(14)	-166.2(5)
C(3)-O(2)-C(2)-O(1)	-6.3(8)
C(3)-O(2)-C(2)-C(1)	174.3(5)
C(9)-C(1)-C(2)-O(1)	103.3(6)
C(13)-C(1)-C(2)-O(1)	-138.8(5)
C(4)-C(1)-C(2)-O(1)	-14.5(7)
C(9)-C(1)-C(2)-O(2)	-77.4(6)
C(13)-C(1)-C(2)-O(2)	40.6(6)
C(4)-C(1)-C(2)-O(2)	164.9(5)
C(7)-N(1)-C(4)-C(1)	-53.5(7)
C(5)-N(1)-C(4)-C(1)	-175.4(5)
C(9)-C(1)-C(4)-N(1)	54.8(6)
C(2)-C(1)-C(4)-N(1)	173.8(5)
C(13)-C(1)-C(4)-N(1)	-63.6(6)
C(4)-N(1)-C(5)-C(6)	-73.7(9)
C(7)-N(1)-C(5)-C(6)	163.2(8)
C(4)-N(1)-C(7)-C(8)	55.3(7)
C(5)-N(1)-C(7)-C(8)	176.9(6)
N(1)-C(7)-C(8)-C(9)	-58.0(7)
N(1)-C(7)-C(8)-C(10)	61.2(7)
N(3)-N(2)-C(9)-C(8)	1.0(10)
N(3)-N(2)-C(9)-C(1)	-179.4(5)
C(7)-C(8)-C(9)-N(2)	-119.8(7)
C(10)-C(8)-C(9)-N(2)	117.0(7)
C(7)-C(8)-C(9)-C(1)	60.6(6)
C(10)-C(8)-C(9)-C(1)	-62.6(6)
C(2)-C(1)-C(9)-N(2)	3.6(7)
C(13)-C(1)-C(9)-N(2)	-116.5(6)
C(4)-C(1)-C(9)-N(2)	121.3(6)
C(2)-C(1)-C(9)-C(8)	-176.7(5)
C(13)-C(1)-C(9)-C(8)	63.2(6)
C(4)-C(1)-C(9)-C(8)	-59.1(6)

C(9)-C(8)-C(10)-C(11)	52.6(8)
C(7)-C(8)-C(10)-C(11)	-66.7(8)
C(8)-C(10)-C(11)-C(13)	-45.4(9)
C(8)-C(10)-C(11)-C(12)	-170.8(6)
C(10)-C(11)-C(13)-C(1)	46.4(9)
C(12)-C(11)-C(13)-C(1)	171.9(6)
C(9)-C(1)-C(13)-C(11)	-54.1(7)
C(2)-C(1)-C(13)-C(11)	-173.9(5)
C(4)-C(1)-C(13)-C(11)	65.0(7)
N(2)-N(3)-C(14)-C(15)	-171.1(5)
N(2)-N(3)-C(14)-C(19)	9.4(7)
N(3)-C(14)-C(15)-C(16)	177.2(5)
C(19)-C(14)-C(15)-C(16)	-3.3(8)
N(3)-C(14)-C(15)-N(4)	-4.5(8)
C(19)-C(14)-C(15)-N(4)	175.0(5)
O(4)-N(4)-C(15)-C(16)	-7.1(8)
O(3)-N(4)-C(15)-C(16)	170.9(5)
O(4)-N(4)-C(15)-C(14)	174.5(6)
O(3)-N(4)-C(15)-C(14)	-7.6(8)
C(14)-C(15)-C(16)-C(17)	1.4(8)
N(4)-C(15)-C(16)-C(17)	-177.0(5)
C(15)-C(16)-C(17)-C(18)	2.0(8)
C(15)-C(16)-C(17)-N(5)	-177.9(5)
O(6)-N(5)-C(17)-C(16)	-165.3(5)
O(5)-N(5)-C(17)-C(16)	14.8(8)
O(6)-N(5)-C(17)-C(18)	14.9(8)
O(5)-N(5)-C(17)-C(18)	-165.1(5)
C(16)-C(17)-C(18)-C(19)	-3.2(9)
N(5)-C(17)-C(18)-C(19)	176.6(5)
C(17)-C(18)-C(19)-C(14)	1.2(9)
N(3)-C(14)-C(19)-C(18)	-178.5(6)
C(15)-C(14)-C(19)-C(18)	2.0(8)
C(29)-N(22)-N(23)-C(34)	168.6(5)
C(23)-O(22)-C(22)-O(21)	5.2(8)
C(23)-O(22)-C(22)-C(21)	-173.9(5)
C(29)-C(21)-C(22)-O(21)	-100.8(6)
C(24)-C(21)-C(22)-O(21)	17.2(7)
C(33)-C(21)-C(22)-O(21)	141.4(5)
C(29)-C(21)-C(22)-O(22)	78.2(6)

C(24)-C(21)-C(22)-O(22)	-163.7(4)
C(33)-C(21)-C(22)-O(22)	-39.5(6)
C(27)-N(21)-C(24)-C(21)	54.6(7)
C(25)-N(21)-C(24)-C(21)	178.1(6)
C(29)-C(21)-C(24)-N(21)	-55.3(6)
C(22)-C(21)-C(24)-N(21)	-174.5(5)
C(33)-C(21)-C(24)-N(21)	63.0(6)
C(27)-N(21)-C(25)-C(26)	-158.8(7)
C(24)-N(21)-C(25)-C(26)	77.4(8)
C(24)-N(21)-C(27)-C(28)	-55.0(7)
C(25)-N(21)-C(27)-C(28)	-178.0(6)
N(21)-C(27)-C(28)-C(29)	56.8(7)
N(21)-C(27)-C(28)-C(30)	-61.1(7)
N(23)-N(22)-C(29)-C(28)	-3.5(9)
N(23)-N(22)-C(29)-C(21)	-178.8(5)
C(30)-C(28)-C(29)-N(22)	-112.6(7)
C(27)-C(28)-C(29)-N(22)	125.1(7)
C(30)-C(28)-C(29)-C(21)	63.0(6)
C(27)-C(28)-C(29)-C(21)	-59.4(6)
C(22)-C(21)-C(29)-N(22)	-7.0(7)
C(24)-C(21)-C(29)-N(22)	-125.0(6)
C(33)-C(21)-C(29)-N(22)	112.8(6)
C(22)-C(21)-C(29)-C(28)	176.8(5)
C(24)-C(21)-C(29)-C(28)	58.8(6)
C(33)-C(21)-C(29)-C(28)	-63.4(6)
C(29)-C(28)-C(30)-C(31)	-53.5(8)
C(27)-C(28)-C(30)-C(31)	65.2(7)
C(28)-C(30)-C(31)-C(33)	46.3(9)
C(28)-C(30)-C(31)-C(32)	170.0(6)
C(30)-C(31)-C(33)-C(21)	-45.8(8)
C(32)-C(31)-C(33)-C(21)	-170.7(6)
C(29)-C(21)-C(33)-C(31)	53.1(7)
C(22)-C(21)-C(33)-C(31)	172.7(5)
C(24)-C(21)-C(33)-C(31)	-66.0(6)
N(22)-N(23)-C(34)-C(35)	171.8(5)
N(22)-N(23)-C(34)-C(39)	-9.0(7)
N(23)-C(34)-C(35)-C(36)	-176.3(5)
C(39)-C(34)-C(35)-C(36)	4.5(8)
N(23)-C(34)-C(35)-N(24)	4.0(8)

C(39)-C(34)-C(35)-N(24)	-175.2(5)
O(24)-N(24)-C(35)-C(36)	5.5(8)
O(23)-N(24)-C(35)-C(36)	-172.3(5)
O(24)-N(24)-C(35)-C(34)	-174.8(6)
O(23)-N(24)-C(35)-C(34)	7.4(8)
C(34)-C(35)-C(36)-C(37)	-2.4(8)
N(24)-C(35)-C(36)-C(37)	177.3(5)
C(35)-C(36)-C(37)-C(38)	-2.2(8)
C(35)-C(36)-C(37)-N(25)	177.6(5)
O(25)-N(25)-C(37)-C(36)	-14.9(8)
O(26)-N(25)-C(37)-C(36)	165.8(5)
O(25)-N(25)-C(37)-C(38)	165.0(5)
O(26)-N(25)-C(37)-C(38)	-14.3(8)
C(36)-C(37)-C(38)-C(39)	4.6(8)
N(25)-C(37)-C(38)-C(39)	-175.2(5)
C(37)-C(38)-C(39)-C(34)	-2.3(8)
N(23)-C(34)-C(39)-C(38)	178.7(5)
C(35)-C(34)-C(39)-C(38)	-2.1(8)

e17phar4: 1-(2,4-dinitrophenyl)-2-(propan-2-ylidene)hydrazine

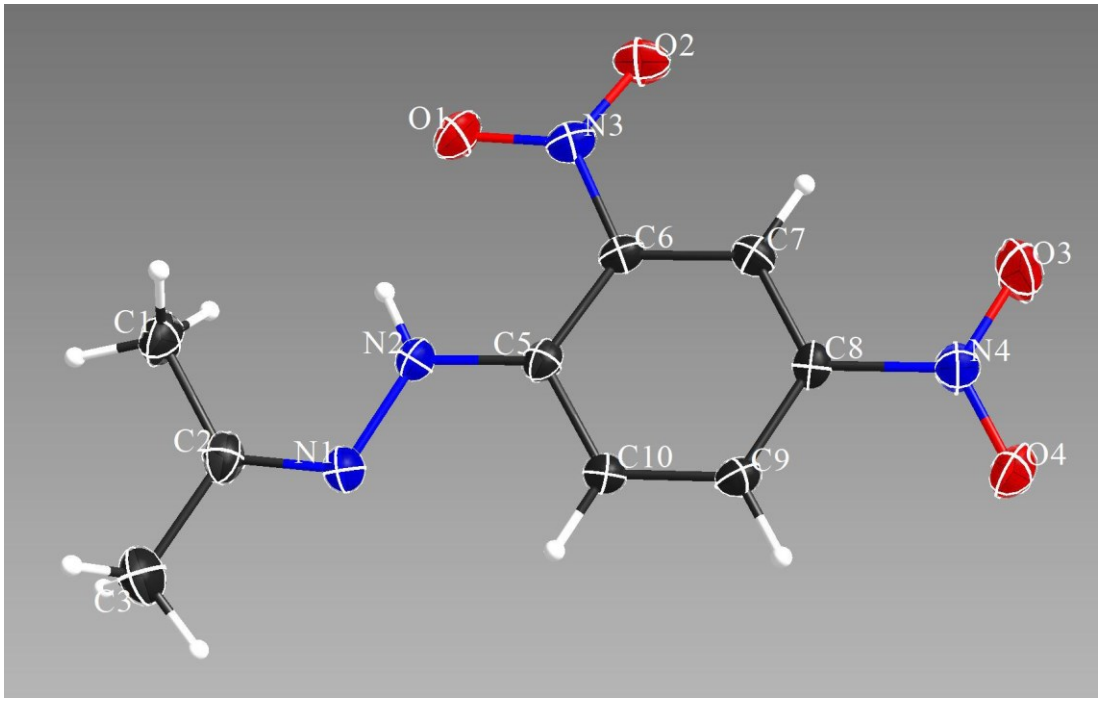

Table 24. Crystal data and structure refinement for e17phar4.

Identification code	e17phar4	
Empirical formula	C9 H10 N4 O4	
Formula weight	238.21	
Temperature	150.01(10) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.1100(4) Å	α= 66.628(5)°.
	b = 8.2112(5) Å	β= 88.929(4)°.
	c = 10.0600(6) Å	γ = 77.803(5)°.
Volume	525.57(6) $Å^3$	
Z	2	
Density (calculated)	1.505 Mg/m^3	
Absorption coefficient	0.121 mm^{-1}	
F(000)	248	
Crystal size	0.500 x 0.400 x 0.060 mm^3	
Theta range for data collection	3.548 to 29.443°.	
Index ranges	-9<=h<=9, -10<=k<=11, -13<=l<=13	
Reflections collected	11559	
Independent reflections	2609 [R(int) = 0.0332]	
Completeness to theta = 25.242°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.86220	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2609 / 0 / 160	
Goodness-of-fit on F^2	1.054	
Final R indices [I>2sigma(I)]	R1 = 0.0491, wR2 = 0.1136	
R indices (all data)	R1 = 0.0685, wR2 = 0.1228	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.341 and -0.239 $e.Å^{-3}$	

Table 25. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for e17phar4. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	7990(2)	4297(2)	3547(1)	33(1)

O(2)	6807(2)	4712(2)	1450(1)	33(1)
O(3)	1491(2)	2346(2)	909(1)	43(1)
O(4)	-15(2)	989(2)	2768(1)	30(1)
N(1)	6002(2)	2155(2)	7360(1)	23(1)
N(2)	6313(2)	2764(2)	5895(1)	22(1)
N(3)	6775(2)	4133(2)	2767(1)	24(1)
N(4)	1252(2)	1807(2)	2201(1)	24(1)
C(1)	9061(2)	2995(2)	7647(2)	28(1)
C(2)	7296(2)	2277(2)	8168(2)	23(1)
C(3)	6999(3)	1623(3)	9752(2)	36(1)
C(5)	5076(2)	2602(2)	4974(2)	18(1)
C(6)	5265(2)	3215(2)	3456(2)	19(1)
C(7)	4005(2)	2963(2)	2548(2)	19(1)
C(8)	2551(2)	2106(2)	3143(2)	19(1)
C(9)	2283(2)	1521(2)	4624(2)	21(1)
C(10)	3510(2)	1770(2)	5517(2)	20(1)

Table 26. Bond lengths [Å] for e17phar4.

O(1)-N(3)	1.2404(17)
O(2)-N(3)	1.2188(16)
O(3)-N(4)	1.2164(17)
O(4)-N(4)	1.2332(17)
N(1)-C(2)	1.2845(19)
N(1)-N(2)	1.3857(17)
N(2)-C(5)	1.3519(18)
N(2)-H(2)	0.85(2)
N(3)-C(6)	1.4493(18)
N(4)-C(8)	1.4577(18)
C(1)-C(2)	1.497(2)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(2)-C(3)	1.493(2)
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800

C(5)-C(10)	1.417(2)
C(5)-C(6)	1.4194(19)
C(6)-C(7)	1.392(2)
C(7)-C(8)	1.368(2)
C(7)-H(7)	0.9500
C(8)-C(9)	1.395(2)
C(9)-C(10)	1.365(2)
C(9)-H(9)	0.9500
C(10)-H(10)	0.9500

Table 27. Bond angles [°] for e17phar4.

C(2)-N(1)-N(2)	115.36(13)
C(5)-N(2)-N(1)	119.40(13)
C(5)-N(2)-H(2)	117.0(13)
N(1)-N(2)-H(2)	123.6(13)
O(2)-N(3)-O(1)	122.50(13)
O(2)-N(3)-C(6)	119.07(12)
O(1)-N(3)-C(6)	118.43(12)
O(3)-N(4)-O(4)	123.57(13)
O(3)-N(4)-C(8)	118.66(13)
O(4)-N(4)-C(8)	117.77(12)
C(2)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
N(1)-C(2)-C(3)	116.44(14)
N(1)-C(2)-C(1)	125.19(14)
C(3)-C(2)-C(1)	118.37(13)
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5

N(2)-C(5)-C(10)	119.87(13)
N(2)-C(5)-C(6)	123.22(13)
C(10)-C(5)-C(6)	116.91(12)
C(7)-C(6)-C(5)	121.59(13)
C(7)-C(6)-N(3)	116.42(13)
C(5)-C(6)-N(3)	121.99(13)
C(8)-C(7)-C(6)	118.81(13)
C(8)-C(7)-H(7)	120.6
C(6)-C(7)-H(7)	120.6
C(7)-C(8)-C(9)	121.54(13)
C(7)-C(8)-N(4)	118.98(13)
C(9)-C(8)-N(4)	119.48(13)
C(10)-C(9)-C(8)	119.87(13)
C(10)-C(9)-H(9)	120.1
C(8)-C(9)-H(9)	120.1
C(9)-C(10)-C(5)	121.25(13)
C(9)-C(10)-H(10)	119.4
C(5)-C(10)-H(10)	119.4

Table 28. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for e17phar4. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	24(1)	46(1)	33(1)	-15(1)	4(1)	-20(1)
O(2)	36(1)	41(1)	24(1)	-9(1)	11(1)	-19(1)
O(3)	50(1)	64(1)	20(1)	-14(1)	-1(1)	-30(1)
O(4)	27(1)	35(1)	31(1)	-13(1)	1(1)	-17(1)
N(1)	22(1)	27(1)	21(1)	-11(1)	1(1)	-7(1)
N(2)	19(1)	29(1)	21(1)	-11(1)	2(1)	-10(1)
N(3)	21(1)	25(1)	26(1)	-9(1)	6(1)	-7(1)
N(4)	26(1)	28(1)	22(1)	-10(1)	-1(1)	-9(1)
C(1)	23(1)	35(1)	33(1)	-18(1)	-2(1)	-8(1)
C(2)	22(1)	24(1)	27(1)	-14(1)	-2(1)	-2(1)
C(3)	36(1)	49(1)	27(1)	-19(1)	-1(1)	-13(1)
C(5)	16(1)	18(1)	22(1)	-10(1)	1(1)	-2(1)
C(6)	17(1)	18(1)	21(1)	-7(1)	4(1)	-5(1)

C(7)	21(1)	20(1)	17(1)	-7(1)	2(1)	-4(1)
C(8)	19(1)	20(1)	20(1)	-8(1)	-2(1)	-4(1)
C(9)	18(1)	23(1)	22(1)	-8(1)	4(1)	-8(1)
C(10)	19(1)	25(1)	18(1)	-8(1)	3(1)	-6(1)

Table 29. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for e17phar4.

	x	y	z	U(eq)
H(1A)	9743	3072	8451	43
H(1B)	8685	4208	6860	43
H(1C)	9912	2174	7290	43
H(3A)	7036	2591	10081	53
H(3B)	8024	556	10291	53
H(3C)	5744	1292	9924	53
H(7)	4152	3380	1535	23
H(9)	1248	950	5009	25
H(10)	3311	1379	6523	24
H(2)	7240(30)	3250(30)	5530(20)	40(6)

Table 30. Torsion angles [°] for e17phar4.

C(2)-N(1)-N(2)-C(5)	176.67(13)
N(2)-N(1)-C(2)-C(3)	-179.73(13)
N(2)-N(1)-C(2)-C(1)	-0.5(2)
N(1)-N(2)-C(5)-C(10)	-1.7(2)
N(1)-N(2)-C(5)-C(6)	178.90(13)
N(2)-C(5)-C(6)-C(7)	177.55(14)
C(10)-C(5)-C(6)-C(7)	-1.9(2)
N(2)-C(5)-C(6)-N(3)	-2.4(2)
C(10)-C(5)-C(6)-N(3)	178.20(12)
O(2)-N(3)-C(6)-C(7)	3.8(2)
O(1)-N(3)-C(6)-C(7)	-176.19(13)
O(2)-N(3)-C(6)-C(5)	-176.30(13)

O(1)-N(3)-C(6)-C(5)	3.7(2)
C(5)-C(6)-C(7)-C(8)	0.1(2)
N(3)-C(6)-C(7)-C(8)	-179.93(13)
C(6)-C(7)-C(8)-C(9)	1.5(2)
C(6)-C(7)-C(8)-N(4)	-178.78(13)
O(3)-N(4)-C(8)-C(7)	-0.7(2)
O(4)-N(4)-C(8)-C(7)	178.15(13)
O(3)-N(4)-C(8)-C(9)	179.08(14)
O(4)-N(4)-C(8)-C(9)	-2.1(2)
C(7)-C(8)-C(9)-C(10)	-1.3(2)
N(4)-C(8)-C(9)-C(10)	179.01(14)
C(8)-C(9)-C(10)-C(5)	-0.6(2)
N(2)-C(5)-C(10)-C(9)	-177.34(14)
C(6)-C(5)-C(10)-C(9)	2.1(2)

Table 31. Hydrogen bonds for e17phar4 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2)...O(1)	0.85(2)	1.95(2)	2.5990(17)	132.8(18)

s17phar15: methyl (1*R*,6*R*,*E*)-10-(2-(2,4-dinitrophenyl)hydrazinylidene)-8-ethyl-8-azabicyclo[4.3.1]decane-1-carboxylate (**19a**) and methyl (1*S*,6*S*,*E*)-10-(2-(2,4-dinitrophenyl)hydrazinylidene)-8-ethyl-8-azabicyclo [4.3.1]decane-1-carboxylate (twin-packed) and (**19b**)

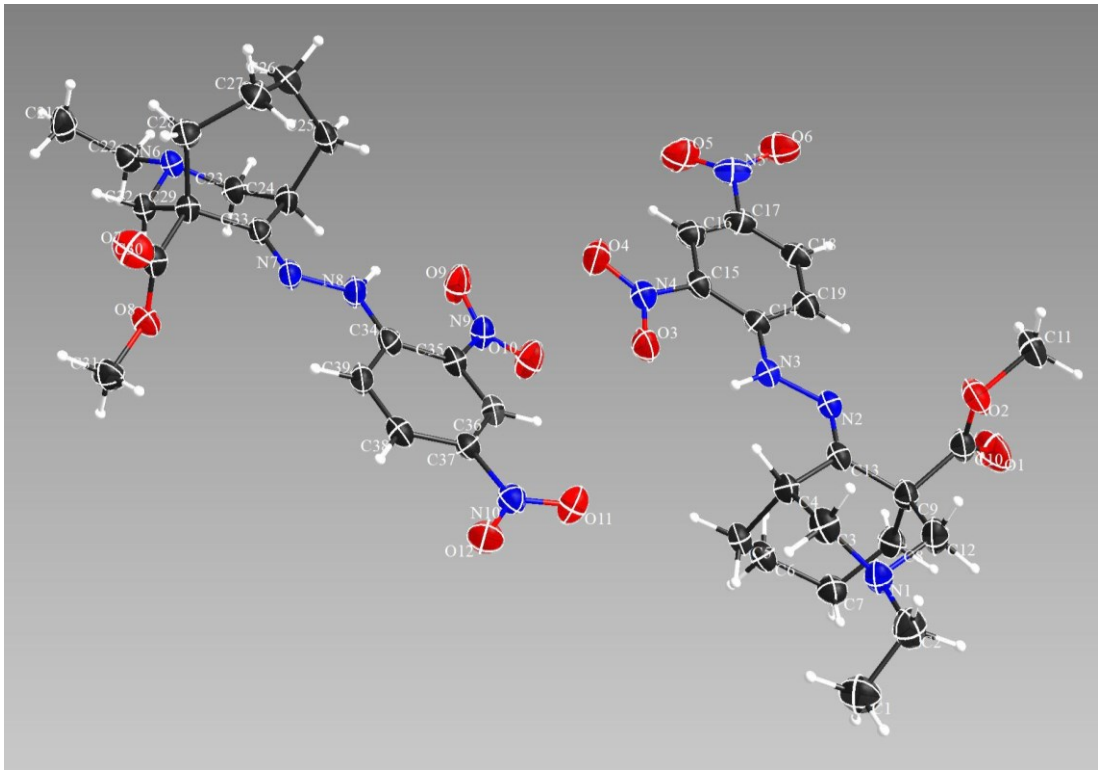

Table 32. Crystal data and structure refinement for s17phar15.

Identification code	s17phar15	
Empirical formula	C19 H25 N5 O6	
Formula weight	419.44	
Temperature	150.01(10) K	
Wavelength	1.54184 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.2535(2) Å	α= 100.206(3)°.
	b = 14.1548(4) Å	β= 99.075(3)°.
	c = 18.1606(7) Å	γ = 102.165(2)°.
Volume	1998.79(11) Å^3	
Z	4	
Density (calculated)	1.394 Mg/m^3	

Absorption coefficient	0.883 mm^{-1}
F(000)	888
Crystal size	0.200 x 0.150 x 0.020 mm^3
Theta range for data collection	3.273 to 72.332°.
Index ranges	-10<=h<=9, -17<=k<=17, -22<=l<=22
Reflections collected	22201
Independent reflections	7805 [R(int) = 0.0391]
Completeness to theta = 67.684°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.73157
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7805 / 0 / 553
Goodness-of-fit on F^2	1.046
Final R indices [I>2sigma(I)]	R1 = 0.0495, wR2 = 0.1240
R indices (all data)	R1 = 0.0703, wR2 = 0.1369
Extinction coefficient	n/a
Largest diff. peak and hole	0.399 and -0.224 e.$Å^{-3}$

Table 33. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for s17phar15. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	1706(2)	4159(1)	1114(1)	34(1)
N(2)	-674(2)	4130(1)	2957(1)	29(1)
N(3)	1(2)	3835(1)	3597(1)	30(1)
N(4)	1485(2)	3395(1)	5030(1)	36(1)
N(5)	-3349(3)	4023(2)	6057(1)	43(1)
O(1)	-3278(2)	4959(2)	1640(1)	60(1)
O(2)	-812(2)	5915(1)	2323(1)	47(1)
O(3)	2249(2)	3292(1)	4494(1)	42(1)
O(4)	2056(2)	3297(1)	5666(1)	50(1)
O(5)	-3013(3)	3574(2)	6553(1)	60(1)
O(6)	-4355(2)	4557(2)	6072(1)	56(1)
C(1)	3483(3)	3691(2)	207(2)	49(1)
C(2)	2719(3)	4481(2)	566(2)	45(1)
C(3)	2751(3)	4266(2)	1867(1)	34(1)

C(4)	1711(2)	3734(1)	2370(1)	28(1)
C(5)	1271(3)	2592(2)	2085(1)	33(1)
C(6)	-572(3)	2075(2)	1746(1)	35(1)
C(7)	-1364(3)	2409(2)	1049(1)	37(1)
C(8)	-2064(3)	3326(2)	1229(1)	37(1)
C(9)	-794(3)	4301(2)	1683(1)	31(1)
C(10)	-1803(3)	5069(2)	1880(1)	36(1)
C(11)	-1644(4)	6702(2)	2507(2)	59(1)
C(12)	446(3)	4723(2)	1204(1)	40(1)
C(13)	125(2)	4091(1)	2406(1)	27(1)
C(14)	-804(3)	3857(1)	4190(1)	29(1)
C(15)	-136(3)	3642(1)	4893(1)	31(1)
C(16)	-978(3)	3683(2)	5500(1)	34(1)
C(17)	-2491(3)	3946(2)	5412(1)	36(1)
C(18)	-3199(3)	4164(2)	4733(1)	36(1)
C(19)	-2381(3)	4118(2)	4134(1)	34(1)
N(6)	6412(2)	-39(1)	8979(1)	26(1)
N(7)	6809(2)	969(1)	6991(1)	30(1)
N(8)	5394(2)	1093(1)	6537(1)	33(1)
N(9)	2399(2)	1263(1)	5541(1)	36(1)
N(10)	5708(2)	1738(1)	3606(1)	32(1)
O(7)	10895(2)	985(1)	7753(1)	46(1)
O(8)	8940(2)	-411(1)	7208(1)	33(1)
O(9)	2297(2)	1280(2)	6211(1)	47(1)
O(10)	1149(2)	1182(2)	5040(1)	48(1)
O(11)	4534(2)	1987(1)	3259(1)	42(1)
O(12)	7008(2)	1685(1)	3365(1)	44(1)
C(21)	7616(3)	-779(2)	10013(1)	42(1)
C(22)	6099(3)	-821(2)	9410(1)	32(1)
C(23)	4845(2)	-72(2)	8459(1)	30(1)
C(24)	5040(2)	715(2)	7972(1)	31(1)
C(25)	4947(3)	1751(2)	8371(1)	39(1)
C(26)	6383(3)	2298(2)	9035(1)	41(1)
C(27)	8133(3)	2500(2)	8837(1)	38(1)
C(28)	9001(3)	1649(2)	8796(1)	33(1)
C(29)	8189(2)	700(1)	8158(1)	26(1)
C(30)	9501(2)	471(2)	7686(1)	29(1)
C(31)	10152(3)	-715(2)	6784(1)	37(1)
C(32)	7682(2)	-188(2)	8529(1)	27(1)

C(33)	6621(2)	794(1)	7645(1)	27(1)
C(34)	5456(3)	1209(1)	5820(1)	29(1)
C(35)	4027(2)	1328(2)	5322(1)	29(1)
C(36)	4113(2)	1490(1)	4603(1)	29(1)
C(37)	5594(3)	1512(1)	4347(1)	28(1)
C(38)	6997(3)	1343(1)	4794(1)	30(1)
C(39)	6931(3)	1199(2)	5515(1)	31(1)

Table 34. Bond lengths [Å] for s17phar15.

N(1)-C(12)	1.450(3)
N(1)-C(3)	1.462(3)
N(1)-C(2)	1.469(3)
N(2)-C(13)	1.282(3)
N(2)-N(3)	1.379(2)
N(3)-C(14)	1.350(3)
N(3)-H(3)	0.85(3)
N(4)-O(4)	1.220(3)
N(4)-O(3)	1.245(2)
N(4)-C(15)	1.449(3)
N(5)-O(5)	1.221(3)
N(5)-O(6)	1.235(3)
N(5)-C(17)	1.461(3)
O(1)-C(10)	1.193(3)
O(2)-C(10)	1.337(3)
O(2)-C(11)	1.444(3)
C(1)-C(2)	1.496(3)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.535(3)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(13)	1.506(3)

C(4)-C(5)	1.553(3)
C(4)-H(4)	1.0000
C(5)-C(6)	1.518(3)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-C(7)	1.529(3)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(8)	1.533(3)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.548(3)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-C(13)	1.519(3)
C(9)-C(10)	1.531(3)
C(9)-C(12)	1.539(3)
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(14)-C(15)	1.419(3)
C(14)-C(19)	1.420(3)
C(15)-C(16)	1.392(3)
C(16)-C(17)	1.370(3)
C(16)-H(16)	0.9500
C(17)-C(18)	1.393(3)
C(18)-C(19)	1.367(3)
C(18)-H(18)	0.9500
C(19)-H(19)	0.9500
N(6)-C(32)	1.454(2)
N(6)-C(23)	1.463(3)
N(6)-C(22)	1.468(2)
N(7)-C(33)	1.282(3)
N(7)-N(8)	1.381(2)
N(8)-C(34)	1.348(3)
N(8)-H(8)	0.87(3)
N(9)-O(9)	1.229(3)

N(9)-O(10)	1.235(2)
N(9)-C(35)	1.451(3)
N(10)-O(11)	1.221(2)
N(10)-O(12)	1.233(2)
N(10)-C(37)	1.450(3)
O(7)-C(30)	1.200(3)
O(8)-C(30)	1.331(3)
O(8)-C(31)	1.444(2)
C(21)-C(22)	1.511(3)
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-C(24)	1.539(3)
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-C(33)	1.509(3)
C(24)-C(25)	1.539(3)
C(24)-H(24)	1.0000
C(25)-C(26)	1.513(3)
C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
C(26)-C(27)	1.524(3)
C(26)-H(26A)	0.9900
C(26)-H(26B)	0.9900
C(27)-C(28)	1.523(3)
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(28)-C(29)	1.556(3)
C(28)-H(28A)	0.9900
C(28)-H(28B)	0.9900
C(29)-C(33)	1.515(3)
C(29)-C(30)	1.535(3)
C(29)-C(32)	1.541(3)
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9900

C(32)-H(32B)	0.9900
C(34)-C(39)	1.416(3)
C(34)-C(35)	1.428(3)
C(35)-C(36)	1.374(3)
C(36)-C(37)	1.371(3)
C(36)-H(36)	0.9500
C(37)-C(38)	1.396(3)
C(38)-C(39)	1.368(3)
C(38)-H(38)	0.9500
C(39)-H(39)	0.9500

Table 35. Bond angles [°] for s17phar15.

C(12)-N(1)-C(3)	108.15(18)
C(12)-N(1)-C(2)	111.05(17)
C(3)-N(1)-C(2)	112.08(18)
C(13)-N(2)-N(3)	117.09(17)
C(14)-N(3)-N(2)	119.18(17)
C(14)-N(3)-H(3)	117.5(18)
N(2)-N(3)-H(3)	123.3(18)
O(4)-N(4)-O(3)	122.29(19)
O(4)-N(4)-C(15)	118.96(19)
O(3)-N(4)-C(15)	118.74(18)
O(5)-N(5)-O(6)	124.0(2)
O(5)-N(5)-C(17)	118.5(2)
O(6)-N(5)-C(17)	117.4(2)
C(10)-O(2)-C(11)	115.7(2)
C(2)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
N(1)-C(2)-C(1)	112.5(2)
N(1)-C(2)-H(2A)	109.1
C(1)-C(2)-H(2A)	109.1

N(1)-C(2)-H(2B)	109.1
C(1)-C(2)-H(2B)	109.1
H(2A)-C(2)-H(2B)	107.8
N(1)-C(3)-C(4)	110.25(17)
N(1)-C(3)-H(3A)	109.6
C(4)-C(3)-H(3A)	109.6
N(1)-C(3)-H(3B)	109.6
C(4)-C(3)-H(3B)	109.6
H(3A)-C(3)-H(3B)	108.1
C(13)-C(4)-C(3)	110.59(16)
C(13)-C(4)-C(5)	110.54(16)
C(3)-C(4)-C(5)	111.71(17)
C(13)-C(4)-H(4)	108.0
C(3)-C(4)-H(4)	108.0
C(5)-C(4)-H(4)	108.0
C(6)-C(5)-C(4)	117.20(17)
C(6)-C(5)-H(5A)	108.0
C(4)-C(5)-H(5A)	108.0
C(6)-C(5)-H(5B)	108.0
C(4)-C(5)-H(5B)	108.0
H(5A)-C(5)-H(5B)	107.2
C(5)-C(6)-C(7)	115.48(18)
C(5)-C(6)-H(6A)	108.4
C(7)-C(6)-H(6A)	108.4
C(5)-C(6)-H(6B)	108.4
C(7)-C(6)-H(6B)	108.4
H(6A)-C(6)-H(6B)	107.5
C(6)-C(7)-C(8)	115.18(19)
C(6)-C(7)-H(7A)	108.5
C(8)-C(7)-H(7A)	108.5
C(6)-C(7)-H(7B)	108.5
C(8)-C(7)-H(7B)	108.5
H(7A)-C(7)-H(7B)	107.5
C(7)-C(8)-C(9)	117.25(18)
C(7)-C(8)-H(8A)	108.0
C(9)-C(8)-H(8A)	108.0
C(7)-C(8)-H(8B)	108.0
C(9)-C(8)-H(8B)	108.0
H(8A)-C(8)-H(8B)	107.2

C(13)-C(9)-C(10)	110.51(18)
C(13)-C(9)-C(12)	111.83(17)
C(10)-C(9)-C(12)	106.91(17)
C(13)-C(9)-C(8)	107.79(16)
C(10)-C(9)-C(8)	107.85(17)
C(12)-C(9)-C(8)	111.88(19)
O(1)-C(10)-O(2)	123.2(2)
O(1)-C(10)-C(9)	124.9(2)
O(2)-C(10)-C(9)	111.82(19)
O(2)-C(11)-H(11A)	109.5
O(2)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
O(2)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
N(1)-C(12)-C(9)	111.90(17)
N(1)-C(12)-H(12A)	109.2
C(9)-C(12)-H(12A)	109.2
N(1)-C(12)-H(12B)	109.2
C(9)-C(12)-H(12B)	109.2
H(12A)-C(12)-H(12B)	107.9
N(2)-C(13)-C(4)	127.15(18)
N(2)-C(13)-C(9)	114.43(17)
C(4)-C(13)-C(9)	117.86(17)
N(3)-C(14)-C(15)	123.04(19)
N(3)-C(14)-C(19)	120.3(2)
C(15)-C(14)-C(19)	116.65(19)
C(16)-C(15)-C(14)	122.0(2)
C(16)-C(15)-N(4)	115.96(19)
C(14)-C(15)-N(4)	122.02(19)
C(17)-C(16)-C(15)	118.6(2)
C(17)-C(16)-H(16)	120.7
C(15)-C(16)-H(16)	120.7
C(16)-C(17)-C(18)	121.6(2)
C(16)-C(17)-N(5)	118.7(2)
C(18)-C(17)-N(5)	119.7(2)
C(19)-C(18)-C(17)	120.0(2)
C(19)-C(18)-H(18)	120.0
C(17)-C(18)-H(18)	120.0

C(18)-C(19)-C(14)	121.2(2)
C(18)-C(19)-H(19)	119.4
C(14)-C(19)-H(19)	119.4
C(32)-N(6)-C(23)	108.44(15)
C(32)-N(6)-C(22)	110.20(15)
C(23)-N(6)-C(22)	109.42(16)
C(33)-N(7)-N(8)	115.84(17)
C(34)-N(8)-N(7)	119.29(18)
C(34)-N(8)-H(8)	117.6(19)
N(7)-N(8)-H(8)	122.9(19)
O(9)-N(9)-O(10)	122.17(19)
O(9)-N(9)-C(35)	119.67(18)
O(10)-N(9)-C(35)	118.16(19)
O(11)-N(10)-O(12)	123.29(19)
O(11)-N(10)-C(37)	118.77(18)
O(12)-N(10)-C(37)	117.92(18)
C(30)-O(8)-C(31)	114.79(16)
C(22)-C(21)-H(21A)	109.5
C(22)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(22)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
N(6)-C(22)-C(21)	112.78(18)
N(6)-C(22)-H(22A)	109.0
C(21)-C(22)-H(22A)	109.0
N(6)-C(22)-H(22B)	109.0
C(21)-C(22)-H(22B)	109.0
H(22A)-C(22)-H(22B)	107.8
N(6)-C(23)-C(24)	113.62(16)
N(6)-C(23)-H(23A)	108.8
C(24)-C(23)-H(23A)	108.8
N(6)-C(23)-H(23B)	108.8
C(24)-C(23)-H(23B)	108.8
H(23A)-C(23)-H(23B)	107.7
C(33)-C(24)-C(23)	112.29(16)
C(33)-C(24)-C(25)	109.78(17)
C(23)-C(24)-C(25)	115.20(18)
C(33)-C(24)-H(24)	106.3

C(23)-C(24)-H(24)	106.3
C(25)-C(24)-H(24)	106.3
C(26)-C(25)-C(24)	116.29(18)
C(26)-C(25)-H(25A)	108.2
C(24)-C(25)-H(25A)	108.2
C(26)-C(25)-H(25B)	108.2
C(24)-C(25)-H(25B)	108.2
H(25A)-C(25)-H(25B)	107.4
C(25)-C(26)-C(27)	115.0(2)
C(25)-C(26)-H(26A)	108.5
C(27)-C(26)-H(26A)	108.5
C(25)-C(26)-H(26B)	108.5
C(27)-C(26)-H(26B)	108.5
H(26A)-C(26)-H(26B)	107.5
C(28)-C(27)-C(26)	116.21(18)
C(28)-C(27)-H(27A)	108.2
C(26)-C(27)-H(27A)	108.2
C(28)-C(27)-H(27B)	108.2
C(26)-C(27)-H(27B)	108.2
H(27A)-C(27)-H(27B)	107.4
C(27)-C(28)-C(29)	118.05(18)
C(27)-C(28)-H(28A)	107.8
C(29)-C(28)-H(28A)	107.8
C(27)-C(28)-H(28B)	107.8
C(29)-C(28)-H(28B)	107.8
H(28A)-C(28)-H(28B)	107.1
C(33)-C(29)-C(30)	110.45(16)
C(33)-C(29)-C(32)	108.28(15)
C(30)-C(29)-C(32)	106.92(15)
C(33)-C(29)-C(28)	112.23(16)
C(30)-C(29)-C(28)	109.59(16)
C(32)-C(29)-C(28)	109.22(17)
O(7)-C(30)-O(8)	122.92(19)
O(7)-C(30)-C(29)	125.6(2)
O(8)-C(30)-C(29)	111.42(16)
O(8)-C(31)-H(31A)	109.5
O(8)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
O(8)-C(31)-H(31C)	109.5

H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
N(6)-C(32)-C(29)	110.55(15)
N(6)-C(32)-H(32A)	109.5
C(29)-C(32)-H(32A)	109.5
N(6)-C(32)-H(32B)	109.5
C(29)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	108.1
N(7)-C(33)-C(24)	127.32(18)
N(7)-C(33)-C(29)	116.06(17)
C(24)-C(33)-C(29)	116.56(17)
N(8)-C(34)-C(39)	121.82(19)
N(8)-C(34)-C(35)	121.80(19)
C(39)-C(34)-C(35)	116.36(19)
C(36)-C(35)-C(34)	121.82(19)
C(36)-C(35)-N(9)	116.47(18)
C(34)-C(35)-N(9)	121.70(19)
C(37)-C(36)-C(35)	119.33(19)
C(37)-C(36)-H(36)	120.3
C(35)-C(36)-H(36)	120.3
C(36)-C(37)-C(38)	121.12(19)
C(36)-C(37)-N(10)	119.14(18)
C(38)-C(37)-N(10)	119.73(18)
C(39)-C(38)-C(37)	119.77(19)
C(39)-C(38)-H(38)	120.1
C(37)-C(38)-H(38)	120.1
C(38)-C(39)-C(34)	121.43(18)
C(38)-C(39)-H(39)	119.3
C(34)-C(39)-H(39)	119.3

Symmetry transformations used to generate equivalent atoms:

Table 36. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for s17phar15. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	35(1)	35(1)	41(1)	16(1)	14(1)	14(1)

N(2)	30(1)	24(1)	34(1)	8(1)	6(1)	9(1)
N(3)	30(1)	28(1)	33(1)	8(1)	6(1)	11(1)
N(4)	42(1)	31(1)	37(1)	9(1)	9(1)	15(1)
N(5)	40(1)	40(1)	42(1)	-1(1)	13(1)	-3(1)
O(1)	41(1)	60(1)	81(2)	6(1)	5(1)	30(1)
O(2)	56(1)	31(1)	60(1)	11(1)	11(1)	23(1)
O(3)	45(1)	47(1)	45(1)	16(1)	14(1)	26(1)
O(4)	56(1)	60(1)	41(1)	20(1)	6(1)	28(1)
O(5)	72(1)	62(1)	48(1)	15(1)	27(1)	11(1)
O(6)	44(1)	70(1)	54(1)	0(1)	20(1)	16(1)
C(1)	46(1)	55(2)	53(2)	12(1)	19(1)	17(1)
C(2)	48(1)	46(1)	55(2)	26(1)	24(1)	18(1)
C(3)	26(1)	33(1)	46(1)	11(1)	10(1)	7(1)
C(4)	26(1)	28(1)	32(1)	8(1)	5(1)	9(1)
C(5)	35(1)	27(1)	41(1)	12(1)	8(1)	15(1)
C(6)	37(1)	26(1)	44(1)	9(1)	9(1)	9(1)
C(7)	36(1)	32(1)	39(1)	4(1)	1(1)	6(1)
C(8)	33(1)	40(1)	36(1)	7(1)	0(1)	14(1)
C(9)	31(1)	32(1)	36(1)	12(1)	7(1)	15(1)
C(10)	39(1)	36(1)	41(1)	17(1)	11(1)	19(1)
C(11)	91(2)	44(2)	60(2)	19(1)	22(2)	44(2)
C(12)	46(1)	41(1)	47(1)	24(1)	19(1)	22(1)
C(13)	27(1)	21(1)	34(1)	6(1)	5(1)	8(1)
C(14)	30(1)	20(1)	35(1)	4(1)	8(1)	4(1)
C(15)	34(1)	22(1)	37(1)	6(1)	7(1)	7(1)
C(16)	39(1)	26(1)	36(1)	5(1)	8(1)	4(1)
C(17)	36(1)	27(1)	40(1)	2(1)	13(1)	1(1)
C(18)	30(1)	32(1)	44(1)	0(1)	9(1)	6(1)
C(19)	30(1)	30(1)	41(1)	5(1)	6(1)	8(1)
N(6)	27(1)	25(1)	31(1)	10(1)	8(1)	10(1)
N(7)	29(1)	26(1)	36(1)	9(1)	2(1)	12(1)
N(8)	31(1)	38(1)	35(1)	13(1)	6(1)	17(1)
N(9)	31(1)	42(1)	41(1)	19(1)	8(1)	15(1)
N(10)	33(1)	29(1)	34(1)	5(1)	6(1)	8(1)
O(7)	34(1)	42(1)	60(1)	7(1)	17(1)	2(1)
O(8)	28(1)	33(1)	40(1)	7(1)	10(1)	11(1)
O(9)	41(1)	74(1)	45(1)	34(1)	19(1)	29(1)
O(10)	29(1)	71(1)	47(1)	24(1)	6(1)	15(1)
O(11)	37(1)	53(1)	39(1)	18(1)	2(1)	11(1)

O(12)	45(1)	57(1)	41(1)	14(1)	19(1)	22(1)
C(21)	46(1)	50(1)	42(1)	26(1)	14(1)	23(1)
C(22)	38(1)	29(1)	35(1)	12(1)	14(1)	11(1)
C(23)	25(1)	30(1)	34(1)	8(1)	7(1)	7(1)
C(24)	26(1)	32(1)	35(1)	10(1)	2(1)	11(1)
C(25)	37(1)	40(1)	48(1)	14(1)	12(1)	23(1)
C(26)	50(1)	36(1)	40(1)	4(1)	7(1)	24(1)
C(27)	44(1)	24(1)	44(1)	5(1)	4(1)	7(1)
C(28)	31(1)	29(1)	35(1)	5(1)	2(1)	6(1)
C(29)	23(1)	25(1)	30(1)	8(1)	5(1)	6(1)
C(30)	27(1)	30(1)	34(1)	12(1)	6(1)	10(1)
C(31)	37(1)	42(1)	38(1)	9(1)	16(1)	16(1)
C(32)	27(1)	29(1)	31(1)	11(1)	7(1)	12(1)
C(33)	28(1)	23(1)	30(1)	7(1)	3(1)	9(1)
C(34)	34(1)	21(1)	33(1)	8(1)	5(1)	10(1)
C(35)	26(1)	28(1)	39(1)	11(1)	9(1)	11(1)
C(36)	26(1)	26(1)	38(1)	9(1)	3(1)	10(1)
C(37)	32(1)	23(1)	29(1)	6(1)	5(1)	8(1)
C(38)	26(1)	24(1)	40(1)	4(1)	8(1)	10(1)
C(39)	29(1)	28(1)	37(1)	8(1)	-1(1)	13(1)

Table 37. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for s17phar15.

	x	y	z	U(eq)
H(3)	910(30)	3630(19)	3639(15)	40(7)
H(1A)	2580	3111	-70	74
H(1B)	4217	3503	606	74
H(1C)	4151	3943	-149	74
H(2A)	3635	5072	833	54
H(2B)	1991	4674	160	54
H(3A)	3184	4977	2114	41
H(3B)	3734	3982	1811	41
H(4)	2411	3903	2899	34

H(5A)	1944	2436	1695	39
H(5B)	1647	2303	2521	39
H(6A)	-1239	2181	2148	42
H(6B)	-668	1354	1601	42
H(7A)	-2296	1855	736	45
H(7B)	-500	2549	736	45
H(8A)	-2966	3169	1521	44
H(8B)	-2604	3447	740	44
H(11A)	-2142	6868	2035	89
H(11B)	-817	7286	2831	89
H(11C)	-2539	6484	2780	89
H(12A)	-196	4717	693	48
H(12B)	1021	5419	1454	48
H(16)	-514	3532	5965	41
H(18)	-4250	4344	4686	44
H(19)	-2877	4264	3672	41
H(8)	4480(40)	1140(20)	6702(16)	50(8)
H(21A)	8476	-1013	9767	62
H(21B)	7268	-1202	10361	62
H(21C)	8087	-95	10301	62
H(22A)	5785	-1474	9050	39
H(22B)	5130	-759	9658	39
H(23A)	3970	21	8761	36
H(23B)	4442	-736	8114	36
H(24)	4065	481	7527	37
H(25A)	4900	2164	7985	47
H(25B)	3873	1684	8558	47
H(26A)	6392	1908	9436	49
H(26B)	6157	2939	9253	49
H(27A)	8033	2693	8337	46
H(27B)	8875	3075	9223	46
H(28A)	9076	1451	9295	39
H(28B)	10174	1906	8736	39
H(31A)	9696	-1402	6501	56
H(31B)	11209	-662	7139	56
H(31C)	10372	-286	6424	56
H(32A)	7226	-800	8126	33
H(32B)	8694	-268	8862	33
H(36)	3155	1586	4287	35

H(38)	7995	1327	4599	36
H(39)	7895	1091	5818	37

Table 38. Torsion angles [°] for s17phar15.

C(13)-N(2)-N(3)-C(14)	-179.52(18)
C(12)-N(1)-C(2)-C(1)	-155.7(2)
C(3)-N(1)-C(2)-C(1)	83.2(3)
C(12)-N(1)-C(3)-C(4)	68.6(2)
C(2)-N(1)-C(3)-C(4)	-168.67(18)
N(1)-C(3)-C(4)-C(13)	-54.2(2)
N(1)-C(3)-C(4)-C(5)	69.4(2)
C(13)-C(4)-C(5)-C(6)	12.3(3)
C(3)-C(4)-C(5)-C(6)	-111.3(2)
C(4)-C(5)-C(6)-C(7)	59.3(3)
C(5)-C(6)-C(7)-C(8)	-85.0(2)
C(6)-C(7)-C(8)-C(9)	61.2(3)
C(7)-C(8)-C(9)-C(13)	-53.7(3)
C(7)-C(8)-C(9)-C(10)	-173.02(19)
C(7)-C(8)-C(9)-C(12)	69.7(2)
C(11)-O(2)-C(10)-O(1)	0.7(4)
C(11)-O(2)-C(10)-C(9)	177.1(2)
C(13)-C(9)-C(10)-O(1)	-126.0(3)
C(12)-C(9)-C(10)-O(1)	112.1(3)
C(8)-C(9)-C(10)-O(1)	-8.4(3)
C(13)-C(9)-C(10)-O(2)	57.7(2)
C(12)-C(9)-C(10)-O(2)	-64.2(2)
C(8)-C(9)-C(10)-O(2)	175.33(18)
C(3)-N(1)-C(12)-C(9)	-64.9(2)
C(2)-N(1)-C(12)-C(9)	171.8(2)
C(13)-C(9)-C(12)-N(1)	47.1(3)
C(10)-C(9)-C(12)-N(1)	168.2(2)
C(8)-C(9)-C(12)-N(1)	-73.9(2)
N(3)-N(2)-C(13)-C(4)	1.5(3)
N(3)-N(2)-C(13)-C(9)	172.74(16)
C(3)-C(4)-C(13)-N(2)	-150.8(2)
C(5)-C(4)-C(13)-N(2)	85.0(2)

C(3)-C(4)-C(13)-C(9)	38.3(2)
C(5)-C(4)-C(13)-C(9)	-85.9(2)
C(10)-C(9)-C(13)-N(2)	34.1(2)
C(12)-C(9)-C(13)-N(2)	153.13(18)
C(8)-C(9)-C(13)-N(2)	-83.5(2)
C(10)-C(9)-C(13)-C(4)	-153.79(18)
C(12)-C(9)-C(13)-C(4)	-34.8(2)
C(8)-C(9)-C(13)-C(4)	88.6(2)
N(2)-N(3)-C(14)-C(15)	-174.95(17)
N(2)-N(3)-C(14)-C(19)	4.0(3)
N(3)-C(14)-C(15)-C(16)	179.05(19)
C(19)-C(14)-C(15)-C(16)	0.0(3)
N(3)-C(14)-C(15)-N(4)	0.9(3)
C(19)-C(14)-C(15)-N(4)	-178.15(18)
O(4)-N(4)-C(15)-C(16)	-4.3(3)
O(3)-N(4)-C(15)-C(16)	175.94(19)
O(4)-N(4)-C(15)-C(14)	174.0(2)
O(3)-N(4)-C(15)-C(14)	-5.8(3)
C(14)-C(15)-C(16)-C(17)	-0.4(3)
N(4)-C(15)-C(16)-C(17)	177.85(18)
C(15)-C(16)-C(17)-C(18)	0.4(3)
C(15)-C(16)-C(17)-N(5)	-177.95(18)
O(5)-N(5)-C(17)-C(16)	-22.3(3)
O(6)-N(5)-C(17)-C(16)	156.4(2)
O(5)-N(5)-C(17)-C(18)	159.3(2)
O(6)-N(5)-C(17)-C(18)	-22.0(3)
C(16)-C(17)-C(18)-C(19)	0.0(3)
N(5)-C(17)-C(18)-C(19)	178.35(19)
C(17)-C(18)-C(19)-C(14)	-0.4(3)
N(3)-C(14)-C(19)-C(18)	-178.7(2)
C(15)-C(14)-C(19)-C(18)	0.4(3)
C(33)-N(7)-N(8)-C(34)	-175.28(18)
C(32)-N(6)-C(22)-C(21)	66.1(2)
C(23)-N(6)-C(22)-C(21)	-174.77(18)
C(32)-N(6)-C(23)-C(24)	-59.2(2)
C(22)-N(6)-C(23)-C(24)	-179.46(17)
N(6)-C(23)-C(24)-C(33)	44.4(2)
N(6)-C(23)-C(24)-C(25)	-82.2(2)
C(33)-C(24)-C(25)-C(26)	-60.9(3)

C(23)-C(24)-C(25)-C(26)	67.1(3)
C(24)-C(25)-C(26)-C(27)	60.3(3)
C(25)-C(26)-C(27)-C(28)	-81.6(3)
C(26)-C(27)-C(28)-C(29)	65.4(3)
C(27)-C(28)-C(29)-C(33)	1.7(3)
C(27)-C(28)-C(29)-C(30)	124.8(2)
C(27)-C(28)-C(29)-C(32)	-118.4(2)
C(31)-O(8)-C(30)-O(7)	1.1(3)
C(31)-O(8)-C(30)-C(29)	-175.54(16)
C(33)-C(29)-C(30)-O(7)	118.3(2)
C(32)-C(29)-C(30)-O(7)	-124.1(2)
C(28)-C(29)-C(30)-O(7)	-5.8(3)
C(33)-C(29)-C(30)-O(8)	-65.1(2)
C(32)-C(29)-C(30)-O(8)	52.5(2)
C(28)-C(29)-C(30)-O(8)	170.78(16)
C(23)-N(6)-C(32)-C(29)	67.6(2)
C(22)-N(6)-C(32)-C(29)	-172.64(17)
C(33)-C(29)-C(32)-N(6)	-60.0(2)
C(30)-C(29)-C(32)-N(6)	-179.01(15)
C(28)-C(29)-C(32)-N(6)	62.5(2)
N(8)-N(7)-C(33)-C(24)	-0.4(3)
N(8)-N(7)-C(33)-C(29)	-177.53(16)
C(23)-C(24)-C(33)-N(7)	144.2(2)
C(25)-C(24)-C(33)-N(7)	-86.2(3)
C(23)-C(24)-C(33)-C(29)	-38.7(2)
C(25)-C(24)-C(33)-C(29)	90.9(2)
C(30)-C(29)-C(33)-N(7)	-20.2(2)
C(32)-C(29)-C(33)-N(7)	-136.91(18)
C(28)-C(29)-C(33)-N(7)	102.5(2)
C(30)-C(29)-C(33)-C(24)	162.43(16)
C(32)-C(29)-C(33)-C(24)	45.7(2)
C(28)-C(29)-C(33)-C(24)	-75.0(2)
N(7)-N(8)-C(34)-C(39)	0.6(3)
N(7)-N(8)-C(34)-C(35)	179.20(18)
N(8)-C(34)-C(35)-C(36)	177.05(19)
C(39)-C(34)-C(35)-C(36)	-4.2(3)
N(8)-C(34)-C(35)-N(9)	-4.3(3)
C(39)-C(34)-C(35)-N(9)	174.46(18)
O(9)-N(9)-C(35)-C(36)	-168.2(2)

O(10)-N(9)-C(35)-C(36)	12.4(3)
O(9)-N(9)-C(35)-C(34)	13.0(3)
O(10)-N(9)-C(35)-C(34)	-166.4(2)
C(34)-C(35)-C(36)-C(37)	1.8(3)
N(9)-C(35)-C(36)-C(37)	-176.92(18)
C(35)-C(36)-C(37)-C(38)	2.0(3)
C(35)-C(36)-C(37)-N(10)	-176.63(18)
O(11)-N(10)-C(37)-C(36)	6.3(3)
O(12)-N(10)-C(37)-C(36)	-174.96(19)
O(11)-N(10)-C(37)-C(38)	-172.35(19)
O(12)-N(10)-C(37)-C(38)	6.4(3)
C(36)-C(37)-C(38)-C(39)	-3.2(3)
N(10)-C(37)-C(38)-C(39)	175.37(18)
C(37)-C(38)-C(39)-C(34)	0.6(3)
N(8)-C(34)-C(39)-C(38)	-178.32(19)
C(35)-C(34)-C(39)-C(38)	3.0(3)

Table 39. Hydrogen bonds for s17phar15 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(3)-H(3)...O(3)	0.85(3)	1.95(3)	2.604(2)	132(2)
N(8)-H(8)...O(9)	0.87(3)	1.94(3)	2.610(2)	133(3)

s18phar3: (1*S*,5*S*)-1-(ethoxycarbonyl)-3-ethyl-9-oxo-3-azabicyclo[3.3.1]nonan-3-ium chloride (**22a**)

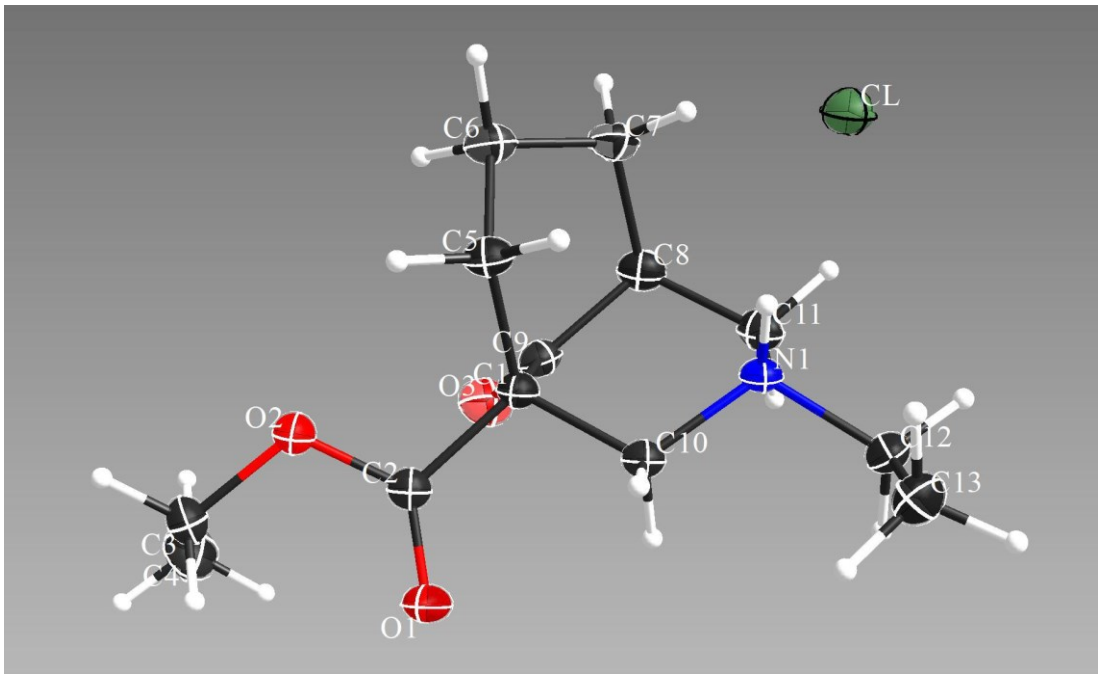

Table 40. Crystal data and structure refinement for s18phar3.

Identification code	s18phar3	
Empirical formula	C13 H22 Cl N O3	
Formula weight	275.76	
Temperature	150.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 14.0556(3) Å	α= 90°.
	b = 8.4265(2) Å	β= 90°.
	c = 23.4225(6) Å	γ = 90°.
Volume	2774.15(11) Å^3	
Z	8	
Density (calculated)	1.321 Mg/m^3	
Absorption coefficient	2.454 mm^{-1}	
F(000)	1184	
Crystal size	0.230 x 0.200 x 0.080 mm^3	

Theta range for data collection	3.774 to 73.497°.
Index ranges	-17<=h<=16, -10<=k<=7, -28<=l<=28
Reflections collected	26135
Independent reflections	2777 [R(int) = 0.0769]
Completeness to theta = 67.684°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.78003
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2777 / 0 / 169
Goodness-of-fit on F^2	1.065
Final R indices [I>2sigma(I)]	R1 = 0.0449, wR2 = 0.1170
R indices (all data)	R1 = 0.0465, wR2 = 0.1185
Extinction coefficient	n/a
Largest diff. peak and hole	0.450 and -0.353 e.$Å^{-3}$

Table 41. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for s18phar3. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	7155(1)	8451(2)	4048(1)	34(1)
O(2)	5779(1)	9125(2)	4465(1)	26(1)
O(3)	6044(1)	5564(2)	4744(1)	31(1)
C(1)	5757(1)	6904(2)	3845(1)	18(1)
C(2)	6317(1)	8246(2)	4120(1)	22(1)
C(3)	6276(1)	10331(2)	4798(1)	28(1)
C(4)	6699(2)	9622(3)	5325(1)	40(1)
C(5)	4727(1)	7380(2)	3658(1)	21(1)
C(6)	3970(1)	6394(2)	3959(1)	24(1)
C(7)	4129(1)	4616(2)	3873(1)	24(1)
C(8)	5168(1)	4134(2)	4020(1)	23(1)
C(9)	5691(1)	5531(2)	4273(1)	21(1)
C(10)	6351(1)	6283(2)	3340(1)	19(1)
N(1)	5930(1)	4831(2)	3074(1)	18(1)
C(11)	5742(1)	3542(2)	3504(1)	23(1)
C(12)	6589(1)	4197(2)	2617(1)	25(1)
C(13)	6707(1)	5332(2)	2122(1)	32(1)

Cl	4146(1)	4968(1)	2318(1)	24(1)

Table 42. Bond lengths [Å] for s18phar3.

O(1)-C(2)	1.202(2)
O(2)-C(2)	1.332(2)
O(2)-C(3)	1.459(2)
O(3)-C(9)	1.208(2)
C(1)-C(2)	1.521(2)
C(1)-C(9)	1.534(2)
C(1)-C(10)	1.540(2)
C(1)-C(5)	1.566(2)
C(3)-C(4)	1.494(3)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(5)-C(6)	1.524(2)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-C(7)	1.529(2)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(8)	1.555(2)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.509(2)
C(8)-C(11)	1.537(2)
C(8)-H(8)	1.0000
C(10)-N(1)	1.4938(19)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
N(1)-C(11)	1.505(2)
N(1)-C(12)	1.514(2)
N(1)-H(1)	0.87(2)
C(11)-H(11A)	0.9900

C(11)-H(11B)	0.9900
C(12)-C(13)	1.513(3)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800

Table 43. Bond angles [°] for s18phar3.

C(2)-O(2)-C(3)	116.13(13)
C(2)-C(1)-C(9)	108.35(13)
C(2)-C(1)-C(10)	107.32(12)
C(9)-C(1)-C(10)	106.22(12)
C(2)-C(1)-C(5)	114.00(13)
C(9)-C(1)-C(5)	108.73(12)
C(10)-C(1)-C(5)	111.89(12)
O(1)-C(2)-O(2)	124.14(15)
O(1)-C(2)-C(1)	123.66(15)
O(2)-C(2)-C(1)	112.16(13)
O(2)-C(3)-C(4)	110.65(15)
O(2)-C(3)-H(3A)	109.5
C(4)-C(3)-H(3A)	109.5
O(2)-C(3)-H(3B)	109.5
C(4)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	108.1
C(3)-C(4)-H(4A)	109.5
C(3)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(3)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(6)-C(5)-C(1)	112.09(13)
C(6)-C(5)-H(5A)	109.2
C(1)-C(5)-H(5A)	109.2
C(6)-C(5)-H(5B)	109.2

C(1)-C(5)-H(5B)	109.2
H(5A)-C(5)-H(5B)	107.9
C(5)-C(6)-C(7)	111.72(14)
C(5)-C(6)-H(6A)	109.3
C(7)-C(6)-H(6A)	109.3
C(5)-C(6)-H(6B)	109.3
C(7)-C(6)-H(6B)	109.3
H(6A)-C(6)-H(6B)	107.9
C(6)-C(7)-C(8)	111.37(14)
C(6)-C(7)-H(7A)	109.4
C(8)-C(7)-H(7A)	109.4
C(6)-C(7)-H(7B)	109.4
C(8)-C(7)-H(7B)	109.4
H(7A)-C(7)-H(7B)	108.0
C(9)-C(8)-C(11)	107.82(13)
C(9)-C(8)-C(7)	109.95(14)
C(11)-C(8)-C(7)	113.79(13)
C(9)-C(8)-H(8)	108.4
C(11)-C(8)-H(8)	108.4
C(7)-C(8)-H(8)	108.4
O(3)-C(9)-C(8)	125.16(15)
O(3)-C(9)-C(1)	123.64(15)
C(8)-C(9)-C(1)	111.16(13)
N(1)-C(10)-C(1)	112.52(12)
N(1)-C(10)-H(10A)	109.1
C(1)-C(10)-H(10A)	109.1
N(1)-C(10)-H(10B)	109.1
C(1)-C(10)-H(10B)	109.1
H(10A)-C(10)-H(10B)	107.8
C(10)-N(1)-C(11)	112.49(12)
C(10)-N(1)-C(12)	109.96(12)
C(11)-N(1)-C(12)	109.04(13)
C(10)-N(1)-H(1)	111.4(13)
C(11)-N(1)-H(1)	108.5(14)
C(12)-N(1)-H(1)	105.2(14)
N(1)-C(11)-C(8)	112.57(13)
N(1)-C(11)-H(11A)	109.1
C(8)-C(11)-H(11A)	109.1
N(1)-C(11)-H(11B)	109.1

C(8)-C(11)-H(11B)	109.1
H(11A)-C(11)-H(11B)	107.8
C(13)-C(12)-N(1)	112.76(14)
C(13)-C(12)-H(12A)	109.0
N(1)-C(12)-H(12A)	109.0
C(13)-C(12)-H(12B)	109.0
N(1)-C(12)-H(12B)	109.0
H(12A)-C(12)-H(12B)	107.8
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5

Table 44. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for s18phar3. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	18(1)	42(1)	41(1)	-16(1)	5(1)	-8(1)
O(2)	19(1)	28(1)	31(1)	-10(1)	0(1)	0(1)
O(3)	30(1)	41(1)	22(1)	4(1)	-6(1)	-1(1)
C(1)	14(1)	21(1)	20(1)	-2(1)	-1(1)	-1(1)
C(2)	19(1)	23(1)	24(1)	-2(1)	0(1)	-1(1)
C(3)	27(1)	24(1)	35(1)	-10(1)	0(1)	-2(1)
C(4)	38(1)	43(1)	41(1)	-11(1)	-13(1)	4(1)
C(5)	15(1)	24(1)	24(1)	1(1)	-1(1)	1(1)
C(6)	16(1)	30(1)	27(1)	1(1)	0(1)	-1(1)
C(7)	17(1)	30(1)	25(1)	2(1)	2(1)	-5(1)
C(8)	21(1)	23(1)	24(1)	5(1)	-1(1)	-2(1)
C(9)	16(1)	27(1)	21(1)	1(1)	0(1)	2(1)
C(10)	15(1)	21(1)	22(1)	-2(1)	0(1)	-1(1)
N(1)	12(1)	21(1)	21(1)	-2(1)	-2(1)	0(1)
C(11)	20(1)	18(1)	30(1)	2(1)	-3(1)	0(1)
C(12)	16(1)	29(1)	29(1)	-9(1)	2(1)	2(1)

C(13)	25(1)	42(1)	27(1)	-7(1)	6(1)	-5(1)
Cl	18(1)	25(1)	29(1)	-2(1)	-4(1)	0(1)

Table 45. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for s18phar3.

	x	y	z	U(eq)
H(3A)	5824	11182	4906	34
H(3B)	6786	10811	4563	34
H(4A)	6196	9122	5552	61
H(4B)	7007	10456	5550	61
H(4C)	7172	8822	5217	61
H(5A)	4622	8517	3744	25
H(5B)	4664	7236	3240	25
H(6A)	3334	6688	3810	29
H(6B)	3981	6637	4373	29
H(7A)	3993	4337	3470	29
H(7B)	3683	4015	4118	29
H(8)	5147	3268	4312	27
H(10A)	6401	7126	3047	23
H(10B)	7002	6036	3474	23
H(1)	5397(16)	5050(20)	2898(9)	23(5)
H(11A)	6357	3109	3640	27
H(11B)	5389	2669	3317	27
H(12A)	7220	3983	2787	30
H(12B)	6333	3179	2472	30
H(13A)	7053	6277	2250	47
H(13B)	6080	5645	1978	47
H(13C)	7066	4811	1816	47

Table 46. Torsion angles [°] for s18phar3.

C(3)-O(2)-C(2)-O(1)	-4.3(3)
C(3)-O(2)-C(2)-C(1)	173.36(14)
C(9)-C(1)-C(2)-O(1)	96.18(19)
C(10)-C(1)-C(2)-O(1)	-18.1(2)
C(5)-C(1)-C(2)-O(1)	-142.62(17)
C(9)-C(1)-C(2)-O(2)	-81.48(16)
C(10)-C(1)-C(2)-O(2)	164.21(13)
C(5)-C(1)-C(2)-O(2)	39.72(18)
C(2)-O(2)-C(3)-C(4)	-82.9(2)
C(2)-C(1)-C(5)-C(6)	-119.53(15)
C(9)-C(1)-C(5)-C(6)	1.47(18)
C(10)-C(1)-C(5)-C(6)	118.46(14)
C(1)-C(5)-C(6)-C(7)	-55.38(18)
C(5)-C(6)-C(7)-C(8)	50.94(18)
C(6)-C(7)-C(8)-C(9)	6.58(18)
C(6)-C(7)-C(8)-C(11)	-114.48(15)
C(11)-C(8)-C(9)-O(3)	-115.31(18)
C(7)-C(8)-C(9)-O(3)	120.12(18)
C(11)-C(8)-C(9)-C(1)	62.39(16)
C(7)-C(8)-C(9)-C(1)	-62.18(16)
C(2)-C(1)-C(9)-O(3)	-0.5(2)
C(10)-C(1)-C(9)-O(3)	114.51(17)
C(5)-C(1)-C(9)-O(3)	-124.93(17)
C(2)-C(1)-C(9)-C(8)	-178.27(13)
C(10)-C(1)-C(9)-C(8)	-63.24(16)
C(5)-C(1)-C(9)-C(8)	57.33(17)
C(2)-C(1)-C(10)-N(1)	173.25(12)
C(9)-C(1)-C(10)-N(1)	57.52(16)
C(5)-C(1)-C(10)-N(1)	-60.98(17)
C(1)-C(10)-N(1)-C(11)	-53.26(17)
C(1)-C(10)-N(1)-C(12)	-174.99(12)
C(10)-N(1)-C(11)-C(8)	51.46(17)
C(12)-N(1)-C(11)-C(8)	173.71(13)
C(9)-C(8)-C(11)-N(1)	-55.06(16)
C(7)-C(8)-C(11)-N(1)	67.18(17)
C(10)-N(1)-C(12)-C(13)	-64.37(17)
C(11)-N(1)-C(12)-C(13)	171.87(13)

Table 47. Hydrogen bonds for s18phar3 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1)...Cl	0.87(2)	2.22(2)	3.0724(14)	163.7(19)

s18phar7: (1*S*,6*S*)-8-ethyl-1-(methoxycarbonyl)-10-oxo-8-azabicyclo[4.3.1]decan-8-ium chloride (**24**)

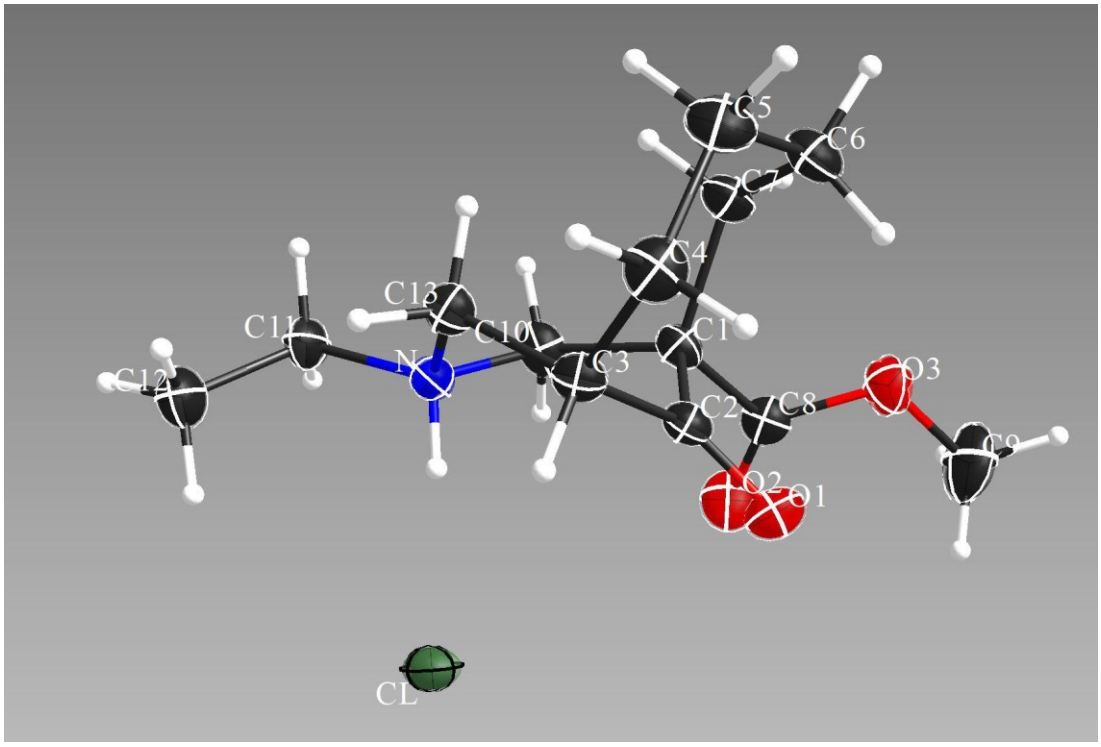

Table 48. Crystal data and structure refinement for s18phar7.

Identification code	s18phar7
Empirical formula	C13 H22 Cl N O3
Formula weight	275.76
Temperature	149.9(3) K
Wavelength	1.54184 Å
Crystal system	Monoclinic
Space group	Cc

Unit cell dimensions	a = 9.8460(3) Å	α= 90°.
	b = 20.9015(6) Å	β= 102.550(3)°.
	c = 6.7809(2) Å	γ = 90°.
Volume	1362.14(7) $Å^3$	
Z	4	
Density (calculated)	1.345 Mg/m^3	
Absorption coefficient	2.498 mm^{-1}	
F(000)	592	
Crystal size	0.200 x 0.100 x 0.040 mm^3	
Theta range for data collection	4.230 to 72.985°.	
Index ranges	-10<=h<=12, -23<=k<=25, -8<=l<=5	
Reflections collected	4159	
Independent reflections	1804 [R(int) = 0.0249]	
Completeness to theta = 67.684°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.66385	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1804 / 2 / 169	
Goodness-of-fit on F^2	1.055	
Final R indices [I>2sigma(I)]	R1 = 0.0326, wR2 = 0.0852	
R indices (all data)	R1 = 0.0332, wR2 = 0.0857	
Absolute structure parameter	-0.02(2)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.467 and -0.247 e.$Å^{-3}$	

Table 49. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for s18phar7. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl	6908(1)	6026(1)	1715(1)	33(1)
N	6706(3)	6131(1)	6041(4)	22(1)
O(1)	3444(2)	6869(1)	2875(3)	28(1)
O(2)	3368(3)	5317(1)	2685(4)	38(1)
O(3)	1723(2)	5828(1)	3911(4)	33(1)
C(1)	4068(3)	6062(1)	5455(5)	21(1)
C(2)	4221(3)	6704(1)	4418(4)	21(1)
C(3)	5360(3)	7138(1)	5540(4)	22(1)

C(4)	4709(3)	7650(1)	6680(5)	28(1)
C(5)	3978(4)	7399(1)	8288(5)	32(1)
C(6)	2896(3)	6869(2)	7609(5)	28(1)
C(7)	3522(3)	6204(1)	7414(5)	24(1)
C(8)	3036(3)	5677(1)	3882(5)	25(1)
C(9)	706(4)	5574(2)	2255(7)	48(1)
C(10)	5477(3)	5702(1)	5978(5)	25(1)
C(11)	8015(3)	5795(2)	7068(5)	27(1)
C(12)	9310(3)	6150(2)	6801(6)	34(1)
C(13)	6522(3)	6768(1)	6938(4)	24(1)

Table 50. Bond lengths [Å] for s18phar7.

N-C(13)	1.491(3)
N-C(10)	1.499(4)
N-C(11)	1.500(4)
N-H	0.91(4)
O(1)-C(2)	1.205(4)
O(2)-C(8)	1.203(4)
O(3)-C(8)	1.335(4)
O(3)-C(9)	1.434(4)
C(1)-C(8)	1.532(4)
C(1)-C(2)	1.537(4)
C(1)-C(10)	1.551(4)
C(1)-C(7)	1.566(4)
C(2)-C(3)	1.513(4)
C(3)-C(13)	1.527(4)
C(3)-C(4)	1.539(4)
C(3)-H(3)	1.0000
C(4)-C(5)	1.524(5)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(6)	1.537(4)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-C(7)	1.537(4)
C(6)-H(6A)	0.9900

C(6)-H(6B)	0.9900
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.521(4)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900

Table 51. Bond angles [°] for s18phar7.

C(13)-N-C(10)	112.1(2)
C(13)-N-C(11)	113.4(2)
C(10)-N-C(11)	109.9(2)
C(13)-N-H	107(2)
C(10)-N-H	105(2)
C(11)-N-H	109(2)
C(8)-O(3)-C(9)	114.5(3)
C(8)-C(1)-C(2)	104.8(2)
C(8)-C(1)-C(10)	109.2(2)
C(2)-C(1)-C(10)	110.9(2)
C(8)-C(1)-C(7)	113.1(2)
C(2)-C(1)-C(7)	108.0(2)
C(10)-C(1)-C(7)	110.7(3)
O(1)-C(2)-C(3)	121.8(2)
O(1)-C(2)-C(1)	122.7(3)
C(3)-C(2)-C(1)	115.4(2)
C(2)-C(3)-C(13)	112.5(2)

C(2)-C(3)-C(4)	109.0(2)
C(13)-C(3)-C(4)	112.2(2)
C(2)-C(3)-H(3)	107.7
C(13)-C(3)-H(3)	107.7
C(4)-C(3)-H(3)	107.7
C(5)-C(4)-C(3)	115.7(2)
C(5)-C(4)-H(4A)	108.4
C(3)-C(4)-H(4A)	108.4
C(5)-C(4)-H(4B)	108.4
C(3)-C(4)-H(4B)	108.4
H(4A)-C(4)-H(4B)	107.4
C(4)-C(5)-C(6)	116.0(2)
C(4)-C(5)-H(5A)	108.3
C(6)-C(5)-H(5A)	108.3
C(4)-C(5)-H(5B)	108.3
C(6)-C(5)-H(5B)	108.3
H(5A)-C(5)-H(5B)	107.4
C(5)-C(6)-C(7)	114.4(3)
C(5)-C(6)-H(6A)	108.7
C(7)-C(6)-H(6A)	108.7
C(5)-C(6)-H(6B)	108.7
C(7)-C(6)-H(6B)	108.7
H(6A)-C(6)-H(6B)	107.6
C(6)-C(7)-C(1)	117.5(2)
C(6)-C(7)-H(7A)	107.9
C(1)-C(7)-H(7A)	107.9
C(6)-C(7)-H(7B)	107.9
C(1)-C(7)-H(7B)	107.9
H(7A)-C(7)-H(7B)	107.2
O(2)-C(8)-O(3)	124.3(3)
O(2)-C(8)-C(1)	124.2(3)
O(3)-C(8)-C(1)	111.3(2)
O(3)-C(9)-H(9A)	109.5
O(3)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
O(3)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
N-C(10)-C(1)	113.1(2)

N-C(10)-H(10A)	109.0
C(1)-C(10)-H(10A)	109.0
N-C(10)-H(10B)	109.0
C(1)-C(10)-H(10B)	109.0
H(10A)-C(10)-H(10B)	107.8
N-C(11)-C(12)	112.0(3)
N-C(11)-H(11A)	109.2
C(12)-C(11)-H(11A)	109.2
N-C(11)-H(11B)	109.2
C(12)-C(11)-H(11B)	109.2
H(11A)-C(11)-H(11B)	107.9
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
N-C(13)-C(3)	109.8(2)
N-C(13)-H(13A)	109.7
C(3)-C(13)-H(13A)	109.7
N-C(13)-H(13B)	109.7
C(3)-C(13)-H(13B)	109.7
H(13A)-C(13)-H(13B)	108.2

Table 52. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for s18phar7. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl	40(1)	40(1)	21(1)	1(1)	8(1)	-2(1)
N	22(1)	24(1)	22(1)	2(1)	7(1)	2(1)
O(1)	32(1)	28(1)	23(1)	2(1)	2(1)	1(1)
O(2)	38(1)	32(1)	43(1)	-16(1)	5(1)	1(1)
O(3)	25(1)	36(1)	37(1)	-6(1)	4(1)	-3(1)
C(1)	23(1)	19(1)	24(1)	-2(1)	7(1)	1(1)
C(2)	22(1)	21(1)	21(1)	-2(1)	9(1)	1(1)

C(3)	24(1)	18(1)	22(1)	2(1)	6(1)	-1(1)
C(4)	32(2)	19(1)	31(2)	-2(1)	6(1)	2(1)
C(5)	38(2)	27(1)	31(2)	-8(1)	11(1)	1(1)
C(6)	28(1)	29(1)	29(2)	-4(1)	14(1)	2(1)
C(7)	28(1)	23(1)	25(1)	1(1)	11(1)	0(1)
C(8)	28(1)	20(1)	27(2)	-1(1)	7(1)	-2(1)
C(9)	33(2)	43(2)	61(3)	-14(2)	-6(2)	-4(2)
C(10)	24(1)	18(1)	35(2)	0(1)	9(1)	-1(1)
C(11)	23(1)	30(1)	28(2)	3(1)	6(1)	6(1)
C(12)	25(2)	40(2)	37(2)	1(1)	7(1)	3(1)
C(13)	24(1)	23(1)	24(1)	1(1)	5(1)	-1(1)

Table 53. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{3}) for s18phar7.

	x	y	z	U(eq)
H	6730(40)	6200(16)	4720(60)	18(8)
H(3)	5779	7362	4512	26
H(4A)	5453	7948	7333	33
H(4B)	4029	7898	5681	33
H(5A)	3509	7763	8797	38
H(5B)	4694	7235	9433	38
H(6A)	2305	6989	6287	33
H(6B)	2288	6842	8594	33
H(7A)	2805	5880	7510	29
H(7B)	4304	6141	8590	29
H(9A)	926	5712	978	72
H(9B)	-218	5733	2331	72
H(9C)	715	5106	2325	72
H(10A)	5570	5492	7309	30
H(10B)	5478	5363	4959	30
H(11A)	8021	5358	6505	32
H(11B)	8031	5754	8528	32
H(12A)	9249	6233	5362	51
H(12B)	10135	5889	7335	51

H(12C)	9382	6557	7534	51
H(13A)	7401	7013	7135	28
H(13B)	6286	6710	8273	28

Table 54. Torsion angles [°] for s18phar7.

C(8)-C(1)-C(2)-O(1)	13.0(4)
C(10)-C(1)-C(2)-O(1)	130.7(3)
C(7)-C(1)-C(2)-O(1)	-107.8(3)
C(8)-C(1)-C(2)-C(3)	-170.9(2)
C(10)-C(1)-C(2)-C(3)	-53.2(3)
C(7)-C(1)-C(2)-C(3)	68.3(3)
O(1)-C(2)-C(3)-C(13)	-158.6(3)
C(1)-C(2)-C(3)-C(13)	25.3(3)
O(1)-C(2)-C(3)-C(4)	76.4(3)
C(1)-C(2)-C(3)-C(4)	-99.8(3)
C(2)-C(3)-C(4)-C(5)	61.9(3)
C(13)-C(3)-C(4)-C(5)	-63.3(3)
C(3)-C(4)-C(5)-C(6)	-51.5(4)
C(4)-C(5)-C(6)-C(7)	76.4(4)
C(5)-C(6)-C(7)-C(1)	-79.7(3)
C(8)-C(1)-C(7)-C(6)	-99.6(3)
C(2)-C(1)-C(7)-C(6)	15.9(4)
C(10)-C(1)-C(7)-C(6)	137.5(3)
C(9)-O(3)-C(8)-O(2)	-6.0(5)
C(9)-O(3)-C(8)-C(1)	169.4(3)
C(2)-C(1)-C(8)-O(2)	91.9(3)
C(10)-C(1)-C(8)-O(2)	-27.0(4)
C(7)-C(1)-C(8)-O(2)	-150.7(3)
C(2)-C(1)-C(8)-O(3)	-83.6(3)
C(10)-C(1)-C(8)-O(3)	157.5(3)
C(7)-C(1)-C(8)-O(3)	33.8(3)
C(13)-N-C(10)-C(1)	38.1(4)
C(11)-N-C(10)-C(1)	165.2(2)
C(8)-C(1)-C(10)-N	135.0(3)
C(2)-C(1)-C(10)-N	19.9(4)

C(7)-C(1)-C(10)-N	-99.9(3)
C(13)-N-C(11)-C(12)	-65.2(3)
C(10)-N-C(11)-C(12)	168.4(3)
C(10)-N-C(13)-C(3)	-67.5(3)
C(11)-N-C(13)-C(3)	167.4(2)
C(2)-C(3)-C(13)-N	33.2(3)
C(4)-C(3)-C(13)-N	156.4(2)

Table 55. Hydrogen bonds for s18phar7 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N-H...Cl	0.91(4)	2.11(4)	2.991(3)	161(3)

s18phar11: ((1*R*,5*S*,9*s*)-9-Hydroxy-3-oxabicyclo[3.3.1]nonane-1,5-diyl) dimethanol (**26**)

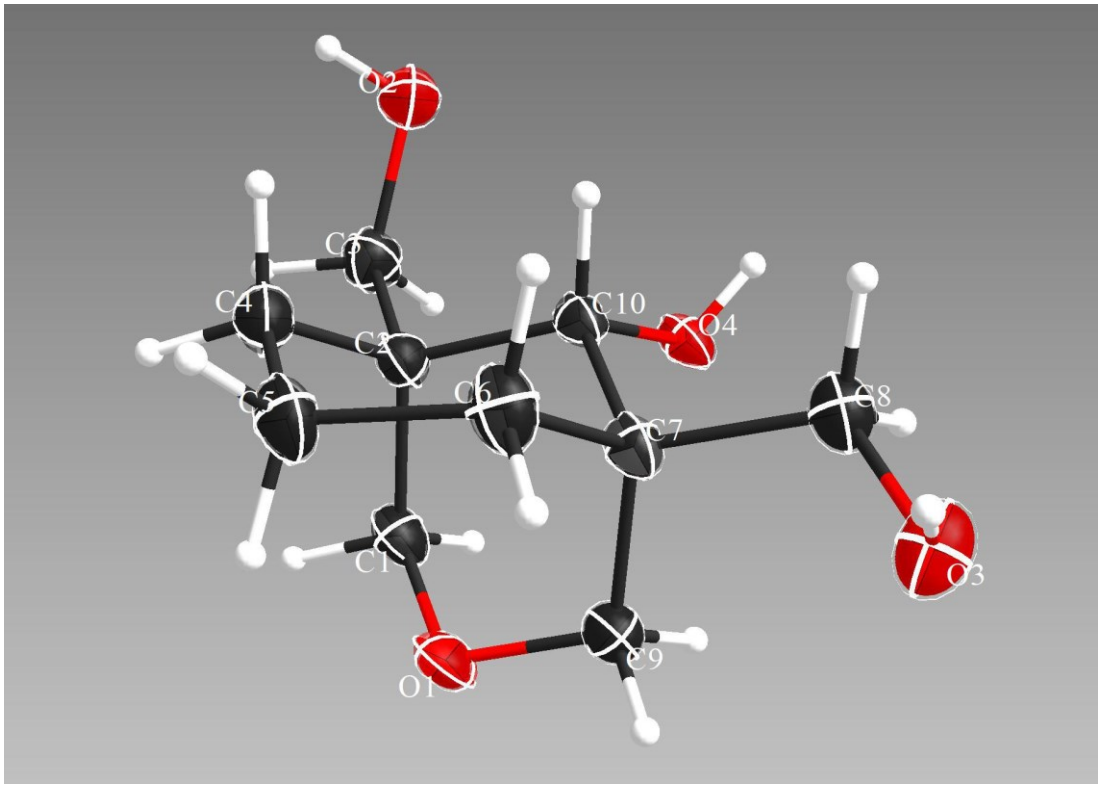

Table 56. Crystal data and structure refinement for s18phar11.

Identification code	s18phar11	
Empirical formula	C10 H18 O4	
Formula weight	202.24	
Temperature	150.01(10) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 5.9795(2) Å	α= 90°.
	b = 10.4226(5) Å	β= 95.080(4)°.
	c = 8.2748(3) Å	γ = 90°.
Volume	513.68(4) $Å^3$	
Z	2	
Density (calculated)	1.308 Mg/m^3	
Absorption coefficient	0.828 mm^{-1}	
F(000)	220	
Crystal size	0.160 x 0.120 x 0.080 mm^3	
Theta range for data collection	5.367 to 73.299°.	
Index ranges	-7<=h<=7, -12<=k<=12, -10<=l<=10	
Reflections collected	7894	
Independent reflections	1990 [R(int) = 0.0342]	
Completeness to theta = 67.684°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.85223	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1990 / 1 / 139	
Goodness-of-fit on F^2	1.052	
Final R indices [I>2sigma(I)]	R1 = 0.0297, wR2 = 0.0764	
R indices (all data)	R1 = 0.0306, wR2 = 0.0773	
Absolute structure parameter	0.12(10)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.220 and -0.153 $e.Å^{-3}$	

Table 57. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for s18phar11. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	9833(2)	4002(2)	6654(2)	28(1)
O(2)	4122(2)	4259(2)	10533(2)	34(1)
O(3)	5403(3)	5881(2)	3033(2)	31(1)
O(4)	4203(2)	3454(1)	6854(2)	23(1)
C(1)	8918(3)	3496(2)	8070(2)	26(1)
C(2)	7146(3)	4382(2)	8702(2)	22(1)
C(3)	6140(3)	3691(2)	10107(2)	29(1)
C(4)	8141(3)	5682(2)	9278(2)	27(1)
C(5)	9013(3)	6503(2)	7940(3)	29(1)
C(6)	7361(3)	6543(2)	6415(2)	27(1)
C(7)	6388(3)	5228(2)	5881(2)	21(1)
C(8)	4565(3)	5397(2)	4469(2)	26(1)
C(9)	8173(3)	4305(2)	5353(2)	25(1)
C(10)	5320(3)	4636(2)	7321(2)	20(1)

Table 58. Bond lengths [Å] for s18phar11.

O(1)-C(9)	1.434(2)
O(1)-C(1)	1.437(2)
O(2)-C(3)	1.416(2)
O(2)-H(2)	0.81(3)
O(3)-C(8)	1.422(2)
O(3)-H(3)	0.81(3)
O(4)-C(10)	1.437(2)
O(4)-H(4)	0.84(3)
C(1)-C(2)	1.532(3)
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(2)-C(10)	1.532(2)
C(2)-C(3)	1.535(3)
C(2)-C(4)	1.538(3)
C(3)-H(3A)	0.9900

C(3)-H(3B)	0.9900
C(4)-C(5)	1.527(3)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(6)	1.533(3)
C(5)-H(5A)	0.9900
C(5)-H(5B)	0.9900
C(6)-C(7)	1.538(3)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(9)	1.530(3)
C(7)-C(10)	1.530(2)
C(7)-C(8)	1.536(2)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-H(10)	1.0000

Table 59. Bond angles [°] for s18phar11.

C(9)-O(1)-C(1)	113.88(13)
C(3)-O(2)-H(2)	107(2)
C(8)-O(3)-H(3)	109.5(17)
C(10)-O(4)-H(4)	104(2)
O(1)-C(1)-C(2)	112.46(17)
O(1)-C(1)-H(1A)	109.1
C(2)-C(1)-H(1A)	109.1
O(1)-C(1)-H(1B)	109.1
C(2)-C(1)-H(1B)	109.1
H(1A)-C(1)-H(1B)	107.8
C(1)-C(2)-C(10)	108.55(14)
C(1)-C(2)-C(3)	107.78(16)
C(10)-C(2)-C(3)	110.18(14)
C(1)-C(2)-C(4)	112.11(15)
C(10)-C(2)-C(4)	108.01(15)

C(3)-C(2)-C(4)	110.20(15)
O(2)-C(3)-C(2)	113.10(17)
O(2)-C(3)-H(3A)	109.0
C(2)-C(3)-H(3A)	109.0
O(2)-C(3)-H(3B)	109.0
C(2)-C(3)-H(3B)	109.0
H(3A)-C(3)-H(3B)	107.8
C(5)-C(4)-C(2)	114.65(16)
C(5)-C(4)-H(4A)	108.6
C(2)-C(4)-H(4A)	108.6
C(5)-C(4)-H(4B)	108.6
C(2)-C(4)-H(4B)	108.6
H(4A)-C(4)-H(4B)	107.6
C(4)-C(5)-C(6)	112.04(16)
C(4)-C(5)-H(5A)	109.2
C(6)-C(5)-H(5A)	109.2
C(4)-C(5)-H(5B)	109.2
C(6)-C(5)-H(5B)	109.2
H(5A)-C(5)-H(5B)	107.9
C(5)-C(6)-C(7)	114.35(16)
C(5)-C(6)-H(6A)	108.7
C(7)-C(6)-H(6A)	108.7
C(5)-C(6)-H(6B)	108.7
C(7)-C(6)-H(6B)	108.7
H(6A)-C(6)-H(6B)	107.6
C(9)-C(7)-C(10)	108.56(15)
C(9)-C(7)-C(8)	108.72(15)
C(10)-C(7)-C(8)	108.77(14)
C(9)-C(7)-C(6)	112.75(15)
C(10)-C(7)-C(6)	108.02(15)
C(8)-C(7)-C(6)	109.94(16)
O(3)-C(8)-C(7)	113.42(15)
O(3)-C(8)-H(8A)	108.9
C(7)-C(8)-H(8A)	108.9
O(3)-C(8)-H(8B)	108.9
C(7)-C(8)-H(8B)	108.9
H(8A)-C(8)-H(8B)	107.7
O(1)-C(9)-C(7)	112.21(15)
O(1)-C(9)-H(9A)	109.2

C(7)-C(9)-H(9A)	109.2
O(1)-C(9)-H(9B)	109.2
C(7)-C(9)-H(9B)	109.2
H(9A)-C(9)-H(9B)	107.9
O(4)-C(10)-C(7)	110.65(14)
O(4)-C(10)-C(2)	109.62(14)
C(7)-C(10)-C(2)	109.38(13)
O(4)-C(10)-H(10)	109.1
C(7)-C(10)-H(10)	109.1
C(2)-C(10)-H(10)	109.1

Table 60. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for s18phar11. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	16(1)	36(1)	33(1)	2(1)	1(1)	4(1)
O(2)	27(1)	45(1)	29(1)	-8(1)	5(1)	-5(1)
O(3)	43(1)	22(1)	26(1)	0(1)	-2(1)	-1(1)
O(4)	15(1)	20(1)	33(1)	-2(1)	-1(1)	-1(1)
C(1)	20(1)	27(1)	32(1)	2(1)	-1(1)	4(1)
C(2)	18(1)	24(1)	24(1)	0(1)	-1(1)	1(1)
C(3)	28(1)	31(1)	26(1)	2(1)	1(1)	0(1)
C(4)	25(1)	28(1)	27(1)	-5(1)	-4(1)	-2(1)
C(5)	25(1)	27(1)	33(1)	-3(1)	-5(1)	-6(1)
C(6)	28(1)	22(1)	31(1)	2(1)	-3(1)	-4(1)
C(7)	19(1)	19(1)	25(1)	-1(1)	-2(1)	-1(1)
C(8)	25(1)	23(1)	27(1)	1(1)	-4(1)	-1(1)
C(9)	20(1)	28(1)	26(1)	-2(1)	2(1)	0(1)
C(10)	16(1)	17(1)	25(1)	-4(1)	-1(1)	1(1)

Table 61. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for s18phar11.

	x	y	z	U(eq)
H(2)	4460(50)	4770(30)	11260(40)	38(7)
H(3)	5430(40)	6660(30)	3070(30)	30(7)
H(4)	2850(60)	3660(30)	6670(30)	44(8)
H(1A)	10149	3367	8936	32
H(1B)	8231	2649	7806	32
H(3A)	5842	2785	9798	35
H(3B)	7252	3696	11068	35
H(4A)	6973	6172	9789	33
H(4B)	9391	5524	10121	33
H(5A)	10466	6153	7655	35
H(5B)	9279	7388	8350	35
H(6A)	8136	6912	5513	33
H(6B)	6106	7124	6617	33
H(8A)	3836	4558	4225	31
H(8B)	3404	5992	4809	31
H(9A)	7436	3503	4944	30
H(9B)	8918	4696	4451	30
H(10)	4200	5251	7706	23

Table 62. Torsion angles [°] for s18phar11.

C(9)-O(1)-C(1)-C(2)	-55.0(2)
O(1)-C(1)-C(2)-C(10)	55.5(2)
O(1)-C(1)-C(2)-C(3)	174.87(15)
O(1)-C(1)-C(2)-C(4)	-63.7(2)
C(1)-C(2)-C(3)-O(2)	-165.30(16)
C(10)-C(2)-C(3)-O(2)	-47.0(2)
C(4)-C(2)-C(3)-O(2)	72.1(2)
C(1)-C(2)-C(4)-C(5)	64.9(2)
C(10)-C(2)-C(4)-C(5)	-54.6(2)
C(3)-C(2)-C(4)-C(5)	-175.05(17)

C(2)-C(4)-C(5)-C(6)	45.4(2)
C(4)-C(5)-C(6)-C(7)	-45.6(2)
C(5)-C(6)-C(7)-C(9)	-64.9(2)
C(5)-C(6)-C(7)-C(10)	55.0(2)
C(5)-C(6)-C(7)-C(8)	173.58(16)
C(9)-C(7)-C(8)-O(3)	-58.8(2)
C(10)-C(7)-C(8)-O(3)	-176.86(15)
C(6)-C(7)-C(8)-O(3)	65.1(2)
C(1)-O(1)-C(9)-C(7)	55.4(2)
C(10)-C(7)-C(9)-O(1)	-56.46(19)
C(8)-C(7)-C(9)-O(1)	-174.64(15)
C(6)-C(7)-C(9)-O(1)	63.2(2)
C(9)-C(7)-C(10)-O(4)	-62.58(17)
C(8)-C(7)-C(10)-O(4)	55.57(18)
C(6)-C(7)-C(10)-O(4)	174.86(14)
C(9)-C(7)-C(10)-C(2)	58.28(18)
C(8)-C(7)-C(10)-C(2)	176.42(15)
C(6)-C(7)-C(10)-C(2)	-64.28(18)
C(1)-C(2)-C(10)-O(4)	63.69(18)
C(3)-C(2)-C(10)-O(4)	-54.11(19)
C(4)-C(2)-C(10)-O(4)	-174.53(14)
C(1)-C(2)-C(10)-C(7)	-57.79(19)
C(3)-C(2)-C(10)-C(7)	-175.59(15)
C(4)-C(2)-C(10)-C(7)	63.99(17)

Table 63. Hydrogen bonds for s18phar11 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(2)-H(2)...O(3)#1	0.81(3)	1.92(3)	2.729(2)	176(3)
O(3)-H(3)...O(4)#2	0.81(3)	1.89(3)	2.694(2)	175(3)
O(4)-H(4)...O(1)#3	0.84(3)	1.84(3)	2.6654(18)	169(3)

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z+1 #2 -x+1,y+1/2,-z+1 #3 x-1,y,z

s17phar9: aconitine (**1b**)

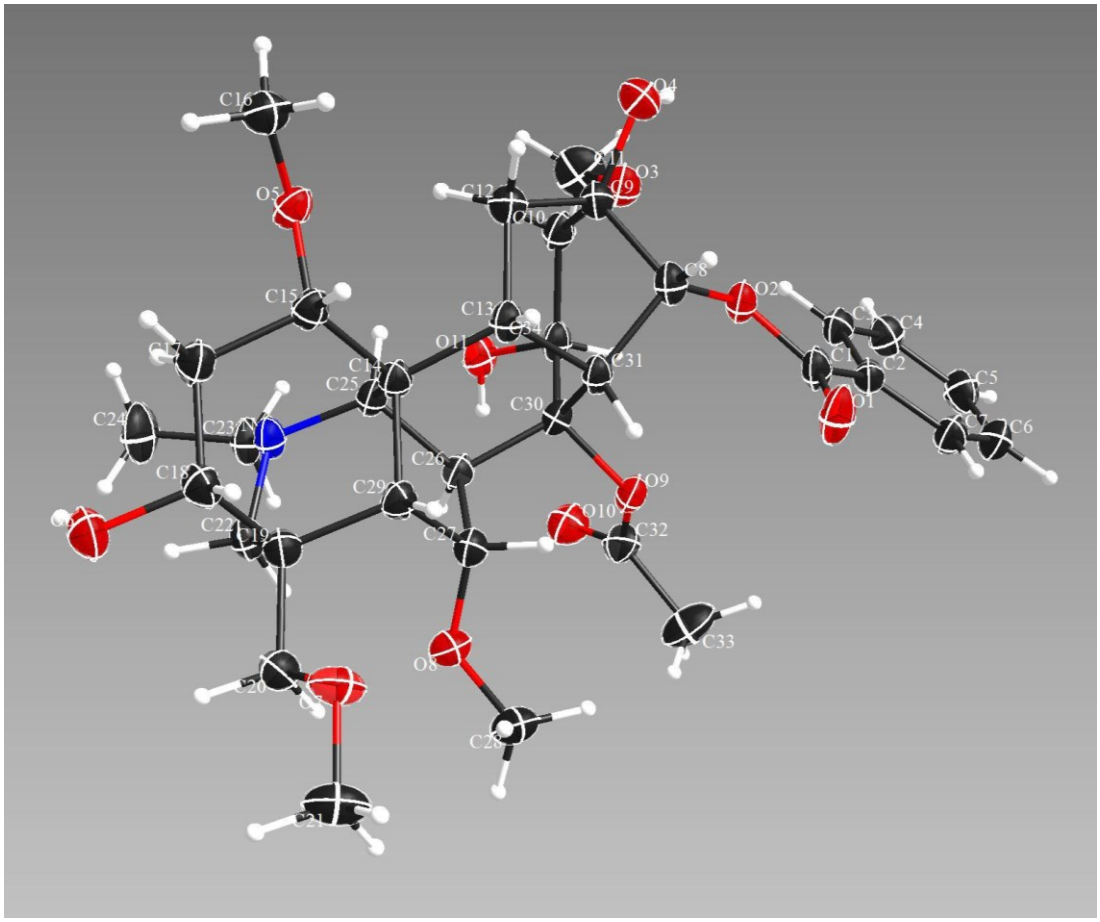

Table 64. Crystal data and structure refinement for s17phar9.

Identification code	s17phar9	
Empirical formula	C34 H47 N O11	
Formula weight	645.72	
Temperature	150.01(10) K	
Wavelength	1.54184 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 12.4482(2) Å	α= 90°.
	b = 15.3388(3) Å	β= 90°.
	c = 16.6801(2) Å	γ = 90°.
Volume	3184.91(9) $Å^3$	
Z	4	
Density (calculated)	1.347 Mg/m^3	
Absorption coefficient	0.829 mm^{-1}	

F(000)	1384
Crystal size	0.300 x 0.280 x 0.080 mm^3
Theta range for data collection	3.915 to 73.355°.
Index ranges	-15<=h<=15, -18<=k<=18, -20<=l<=19
Reflections collected	62398
Independent reflections	6350 [R(int) = 0.0665]
Completeness to theta = 1.000°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.49180
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6350 / 0 / 433
Goodness-of-fit on F^2	1.025
Final R indices [I>2sigma(I)]	R1 = 0.0336, wR2 = 0.0873
R indices (all data)	R1 = 0.0357, wR2 = 0.0887
Absolute structure parameter	-0.05(6)
Extinction coefficient	n/a
Largest diff. peak and hole	0.204 and -0.205 e.$Å^{-3}$

Table 65. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for s17phar9. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3502(2)	4621(2)	2767(1)	26(1)
C(2)	2721(2)	3908(2)	2615(1)	24(1)
C(3)	2120(2)	3537(2)	3234(1)	26(1)
C(4)	1383(2)	2886(2)	3063(1)	31(1)
C(5)	1247(2)	2595(2)	2281(2)	33(1)
C(6)	1833(2)	2975(2)	1664(1)	35(1)
C(7)	2564(2)	3624(2)	1826(1)	31(1)
C(8)	4223(2)	5497(1)	3837(1)	24(1)
C(9)	3992(2)	5664(1)	4721(1)	24(1)
C(10)	3942(2)	4784(2)	5180(1)	25(1)
C(11)	2557(2)	3966(2)	5837(2)	46(1)
C(12)	4981(2)	6187(1)	4973(1)	26(1)
C(13)	5923(2)	5938(1)	4389(1)	22(1)
C(14)	7018(2)	5714(1)	4808(1)	21(1)

C(15)	7365(2)	6519(1)	5307(1)	23(1)
C(16)	6507(2)	7530(2)	6173(1)	31(1)
C(17)	8502(2)	6488(2)	5649(1)	27(1)
C(18)	9328(2)	6171(2)	5057(1)	27(1)
C(19)	8999(2)	5305(1)	4653(1)	25(1)
C(20)	9919(2)	5070(2)	4074(1)	28(1)
C(21)	10738(2)	5529(2)	2871(2)	41(1)
C(22)	8851(2)	4564(1)	5268(1)	26(1)
C(23)	7680(2)	3874(2)	6235(1)	30(1)
C(24)	8372(3)	3902(2)	6978(2)	45(1)
C(25)	6887(2)	4846(1)	5254(1)	22(1)
C(26)	6686(2)	4224(1)	4534(1)	22(1)
C(27)	7460(2)	4554(1)	3869(1)	25(1)
C(28)	8451(2)	3899(2)	2824(2)	46(1)
C(29)	7917(2)	5434(1)	4201(1)	22(1)
C(30)	5538(2)	4301(1)	4218(1)	22(1)
C(31)	5395(2)	5217(1)	3856(1)	21(1)
C(32)	5548(2)	2871(2)	3553(1)	30(1)
C(33)	5687(3)	2471(2)	2738(2)	47(1)
C(34)	4619(2)	4038(1)	4813(1)	23(1)
N	7841(1)	4640(1)	5728(1)	24(1)
O(1)	4067(2)	4965(1)	2271(1)	38(1)
O(2)	3484(1)	4850(1)	3548(1)	25(1)
O(3)	2838(1)	4532(1)	5195(1)	31(1)
O(4)	3050(1)	6157(1)	4856(1)	31(1)
O(5)	6647(1)	6644(1)	5966(1)	26(1)
O(6)	10364(1)	6115(1)	5439(1)	37(1)
O(7)	9897(1)	5678(1)	3425(1)	34(1)
O(8)	8193(1)	3882(1)	3659(1)	32(1)
O(9)	5461(1)	3739(1)	3492(1)	26(1)
O(10)	5528(2)	2464(1)	4173(1)	36(1)
O(11)	4994(1)	3515(1)	5460(1)	30(1)

Table 66. Selected bond lengths [Å] and angles [°] for s17phar9.

C(1)-O(1)	1.208(3)
C(1)-O(2)	1.349(3)
C(1)-C(2)	1.486(3)
C(2)-C(3)	1.396(3)
C(2)-C(7)	1.399(3)
C(3)-C(4)	1.386(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.389(3)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.389(4)
C(5)-H(5)	0.9500
C(6)-C(7)	1.376(4)
C(6)-H(6A)	0.9500
C(7)-H(7)	0.9500
C(8)-O(2)	1.437(3)
C(8)-C(31)	1.520(3)
C(8)-C(9)	1.524(3)
C(8)-H(8)	1.0000
C(9)-O(4)	1.413(3)
C(9)-C(12)	1.529(3)
C(9)-C(10)	1.553(3)
C(10)-O(3)	1.428(3)
C(10)-C(34)	1.548(3)
C(10)-H(10)	1.0000
C(11)-O(3)	1.422(3)
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-C(13)	1.571(3)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(31)	1.565(3)
C(13)-C(14)	1.570(3)
C(13)-H(13)	1.0000
C(14)-C(25)	1.534(3)
C(14)-C(15)	1.550(3)

C(14)-C(29)	1.569(3)
C(15)-O(5)	1.429(2)
C(15)-C(17)	1.527(3)
C(15)-H(15)	1.0000
C(16)-O(5)	1.413(3)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-C(18)	1.506(3)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-O(6)	1.441(3)
C(18)-C(19)	1.544(3)
C(18)-H(18)	1.0000
C(19)-C(20)	1.541(3)
C(19)-C(22)	1.542(3)
C(19)-C(29)	1.555(3)
C(20)-O(7)	1.429(3)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(21)-O(7)	1.415(3)
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-N	1.477(3)
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-N	1.461(3)
C(23)-C(24)	1.510(3)
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-N	1.460(3)
C(25)-C(26)	1.555(3)
C(25)-H(25)	1.0000
C(26)-C(30)	1.528(3)
C(26)-C(27)	1.554(3)

C(26)-H(26)	1.0000
C(27)-O(8)	1.420(3)
C(27)-C(29)	1.566(3)
C(27)-H(27)	1.0000
C(28)-O(8)	1.430(3)
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-H(29)	1.0000
C(30)-O(9)	1.489(2)
C(30)-C(31)	1.540(3)
C(30)-C(34)	1.567(3)
C(31)-H(31)	1.0000
C(32)-O(10)	1.208(3)
C(32)-O(9)	1.339(3)
C(32)-C(33)	1.501(3)
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-O(11)	1.423(2)
C(34)-H(34)	1.0000
O(4)-H(4)	0.87(3)
O(6)-H(6)	0.78(5)
O(11)-H(11)	0.88(4)

Table 67. Bond angles [°] for s17phar9.

O(1)-C(1)-O(2)	123.9(2)
O(1)-C(1)-C(2)	125.8(2)
O(2)-C(1)-C(2)	110.26(17)
C(3)-C(2)-C(7)	119.6(2)
C(3)-C(2)-C(1)	121.58(19)
C(7)-C(2)-C(1)	118.77(19)
C(4)-C(3)-C(2)	119.7(2)
C(4)-C(3)-H(3)	120.1
C(2)-C(3)-H(3)	120.1

C(3)-C(4)-C(5)	120.4(2)
C(3)-C(4)-H(4A)	119.8
C(5)-C(4)-H(4A)	119.8
C(6)-C(5)-C(4)	119.8(2)
C(6)-C(5)-H(5)	120.1
C(4)-C(5)-H(5)	120.1
C(7)-C(6)-C(5)	120.4(2)
C(7)-C(6)-H(6A)	119.8
C(5)-C(6)-H(6A)	119.8
C(6)-C(7)-C(2)	120.1(2)
C(6)-C(7)-H(7)	119.9
C(2)-C(7)-H(7)	119.9
O(2)-C(8)-C(31)	115.21(18)
O(2)-C(8)-C(9)	108.63(17)
C(31)-C(8)-C(9)	102.05(16)
O(2)-C(8)-H(8)	110.2
C(31)-C(8)-H(8)	110.2
C(9)-C(8)-H(8)	110.2
O(4)-C(9)-C(8)	113.63(16)
O(4)-C(9)-C(12)	110.07(17)
C(8)-C(9)-C(12)	101.68(16)
O(4)-C(9)-C(10)	110.70(18)
C(8)-C(9)-C(10)	109.80(17)
C(12)-C(9)-C(10)	110.63(17)
O(3)-C(10)-C(34)	109.37(17)
O(3)-C(10)-C(9)	106.40(17)
C(34)-C(10)-C(9)	115.21(17)
O(3)-C(10)-H(10)	108.6
C(34)-C(10)-H(10)	108.6
C(9)-C(10)-H(10)	108.6
O(3)-C(11)-H(11A)	109.5
O(3)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
O(3)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(9)-C(12)-C(13)	107.64(16)
C(9)-C(12)-H(12A)	110.2
C(13)-C(12)-H(12A)	110.2

C(9)-C(12)-H(12B)	110.2
C(13)-C(12)-H(12B)	110.2
H(12A)-C(12)-H(12B)	108.5
C(31)-C(13)-C(14)	117.56(17)
C(31)-C(13)-C(12)	102.15(16)
C(14)-C(13)-C(12)	115.20(16)
C(31)-C(13)-H(13)	107.1
C(14)-C(13)-H(13)	107.1
C(12)-C(13)-H(13)	107.1
C(25)-C(14)-C(15)	117.37(16)
C(25)-C(14)-C(29)	98.70(15)
C(15)-C(14)-C(29)	111.45(16)
C(25)-C(14)-C(13)	108.31(16)
C(15)-C(14)-C(13)	107.80(16)
C(29)-C(14)-C(13)	113.16(15)
O(5)-C(15)-C(17)	107.23(16)
O(5)-C(15)-C(14)	110.25(16)
C(17)-C(15)-C(14)	115.70(18)
O(5)-C(15)-H(15)	107.8
C(17)-C(15)-H(15)	107.8
C(14)-C(15)-H(15)	107.8
O(5)-C(16)-H(16A)	109.5
O(5)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
O(5)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(18)-C(17)-C(15)	113.46(17)
C(18)-C(17)-H(17A)	108.9
C(15)-C(17)-H(17A)	108.9
C(18)-C(17)-H(17B)	108.9
C(15)-C(17)-H(17B)	108.9
H(17A)-C(17)-H(17B)	107.7
O(6)-C(18)-C(17)	109.94(18)
O(6)-C(18)-C(19)	112.24(18)
C(17)-C(18)-C(19)	112.47(18)
O(6)-C(18)-H(18)	107.3
C(17)-C(18)-H(18)	107.3
C(19)-C(18)-H(18)	107.3

C(20)-C(19)-C(22)	109.41(18)
C(20)-C(19)-C(18)	106.16(17)
C(22)-C(19)-C(18)	112.08(17)
C(20)-C(19)-C(29)	111.66(17)
C(22)-C(19)-C(29)	108.18(17)
C(18)-C(19)-C(29)	109.40(17)
O(7)-C(20)-C(19)	107.92(17)
O(7)-C(20)-H(20A)	110.1
C(19)-C(20)-H(20A)	110.1
O(7)-C(20)-H(20B)	110.1
C(19)-C(20)-H(20B)	110.1
H(20A)-C(20)-H(20B)	108.4
O(7)-C(21)-H(21A)	109.5
O(7)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
O(7)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
N-C(22)-C(19)	112.86(17)
N-C(22)-H(22A)	109.0
C(19)-C(22)-H(22A)	109.0
N-C(22)-H(22B)	109.0
C(19)-C(22)-H(22B)	109.0
H(22A)-C(22)-H(22B)	107.8
N-C(23)-C(24)	112.0(2)
N-C(23)-H(23A)	109.2
C(24)-C(23)-H(23A)	109.2
N-C(23)-H(23B)	109.2
C(24)-C(23)-H(23B)	109.2
H(23A)-C(23)-H(23B)	107.9
C(23)-C(24)-H(24A)	109.5
C(23)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(23)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
N-C(25)-C(14)	111.35(16)
N-C(25)-C(26)	114.57(17)
C(14)-C(25)-C(26)	100.03(15)

N-C(25)-H(25)	110.2
C(14)-C(25)-H(25)	110.2
C(26)-C(25)-H(25)	110.2
C(30)-C(26)-C(27)	107.96(16)
C(30)-C(26)-C(25)	111.71(16)
C(27)-C(26)-C(25)	104.60(16)
C(30)-C(26)-H(26)	110.8
C(27)-C(26)-H(26)	110.8
C(25)-C(26)-H(26)	110.8
O(8)-C(27)-C(26)	109.77(18)
O(8)-C(27)-C(29)	118.61(18)
C(26)-C(27)-C(29)	104.67(16)
O(8)-C(27)-H(27)	107.8
C(26)-C(27)-H(27)	107.8
C(29)-C(27)-H(27)	107.8
O(8)-C(28)-H(28A)	109.5
O(8)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
O(8)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(19)-C(29)-C(27)	112.17(17)
C(19)-C(29)-C(14)	109.87(15)
C(27)-C(29)-C(14)	101.81(16)
C(19)-C(29)-H(29)	110.9
C(27)-C(29)-H(29)	110.9
C(14)-C(29)-H(29)	110.9
O(9)-C(30)-C(26)	107.17(16)
O(9)-C(30)-C(31)	101.64(15)
C(26)-C(30)-C(31)	108.31(16)
O(9)-C(30)-C(34)	108.60(15)
C(26)-C(30)-C(34)	116.35(16)
C(31)-C(30)-C(34)	113.57(16)
C(8)-C(31)-C(30)	112.10(17)
C(8)-C(31)-C(13)	102.43(16)
C(30)-C(31)-C(13)	111.91(16)
C(8)-C(31)-H(31)	110.1
C(30)-C(31)-H(31)	110.1
C(13)-C(31)-H(31)	110.1

O(10)-C(32)-O(9)	125.2(2)
O(10)-C(32)-C(33)	124.5(2)
O(9)-C(32)-C(33)	110.3(2)
C(32)-C(33)-H(33A)	109.5
C(32)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(32)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
O(11)-C(34)-C(10)	107.18(17)
O(11)-C(34)-C(30)	112.74(17)
C(10)-C(34)-C(30)	117.20(17)
O(11)-C(34)-H(34)	106.3
C(10)-C(34)-H(34)	106.3
C(30)-C(34)-H(34)	106.3
C(25)-N-C(23)	112.06(16)
C(25)-N-C(22)	115.39(16)
C(23)-N-C(22)	110.73(17)
C(1)-O(2)-C(8)	119.54(17)
C(11)-O(3)-C(10)	114.51(19)
C(9)-O(4)-H(4)	105.4(19)
C(16)-O(5)-C(15)	113.29(16)
C(18)-O(6)-H(6)	110(4)
C(21)-O(7)-C(20)	112.11(18)
C(27)-O(8)-C(28)	111.8(2)
C(32)-O(9)-C(30)	120.60(16)
C(34)-O(11)-H(11)	112(2)

Symmetry transformations used to generate equivalent atoms:

Table 68. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for s17phar9. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	24(1)	36(1)	19(1)	6(1)	-5(1)	-1(1)
C(2)	21(1)	32(1)	20(1)	1(1)	-3(1)	0(1)

C(3)	28(1)	31(1)	20(1)	3(1)	-2(1)	1(1)
C(4)	30(1)	34(1)	30(1)	8(1)	0(1)	-2(1)
C(5)	30(1)	31(1)	37(1)	0(1)	-8(1)	-4(1)
C(6)	34(1)	43(1)	26(1)	-7(1)	-5(1)	0(1)
C(7)	27(1)	45(1)	20(1)	0(1)	0(1)	-1(1)
C(8)	23(1)	27(1)	21(1)	4(1)	-4(1)	-3(1)
C(9)	22(1)	29(1)	21(1)	-1(1)	-2(1)	2(1)
C(10)	24(1)	34(1)	18(1)	-1(1)	-1(1)	-4(1)
C(11)	40(1)	52(2)	46(2)	15(1)	13(1)	-9(1)
C(12)	24(1)	28(1)	25(1)	-3(1)	-1(1)	1(1)
C(13)	23(1)	24(1)	19(1)	2(1)	-2(1)	-1(1)
C(14)	20(1)	25(1)	17(1)	0(1)	-1(1)	-1(1)
C(15)	24(1)	26(1)	18(1)	-1(1)	2(1)	-3(1)
C(16)	34(1)	31(1)	29(1)	-4(1)	4(1)	3(1)
C(17)	25(1)	32(1)	24(1)	-3(1)	-2(1)	-5(1)
C(18)	20(1)	33(1)	28(1)	-1(1)	-2(1)	-3(1)
C(19)	23(1)	30(1)	23(1)	-1(1)	-1(1)	0(1)
C(20)	24(1)	33(1)	29(1)	1(1)	0(1)	2(1)
C(21)	37(1)	42(1)	43(1)	1(1)	18(1)	6(1)
C(22)	24(1)	30(1)	25(1)	2(1)	-5(1)	1(1)
C(23)	33(1)	34(1)	23(1)	6(1)	-6(1)	-3(1)
C(24)	49(2)	58(2)	30(1)	13(1)	-16(1)	-4(1)
C(25)	23(1)	25(1)	17(1)	-1(1)	-3(1)	-2(1)
C(26)	25(1)	25(1)	17(1)	-1(1)	-2(1)	0(1)
C(27)	24(1)	31(1)	21(1)	-2(1)	-2(1)	1(1)
C(28)	35(1)	70(2)	34(1)	-20(1)	6(1)	5(1)
C(29)	22(1)	27(1)	18(1)	2(1)	0(1)	-1(1)
C(30)	25(1)	24(1)	16(1)	-2(1)	-2(1)	-2(1)
C(31)	21(1)	28(1)	15(1)	3(1)	-2(1)	-3(1)
C(32)	29(1)	30(1)	31(1)	-7(1)	-1(1)	-4(1)
C(33)	63(2)	41(1)	37(1)	-14(1)	8(1)	-8(1)
C(34)	26(1)	27(1)	17(1)	3(1)	-2(1)	-2(1)
N	23(1)	31(1)	20(1)	4(1)	-4(1)	-2(1)
O(1)	38(1)	55(1)	20(1)	8(1)	-4(1)	-17(1)
O(2)	24(1)	34(1)	18(1)	2(1)	-4(1)	-4(1)
O(3)	26(1)	41(1)	27(1)	1(1)	4(1)	-7(1)
O(4)	24(1)	36(1)	34(1)	-2(1)	0(1)	2(1)
O(5)	28(1)	29(1)	19(1)	-3(1)	3(1)	-4(1)
O(6)	24(1)	50(1)	36(1)	-4(1)	-6(1)	-6(1)

O(7)	31(1)	38(1)	32(1)	4(1)	12(1)	8(1)
O(8)	31(1)	36(1)	30(1)	-9(1)	2(1)	3(1)
O(9)	28(1)	30(1)	18(1)	-4(1)	-3(1)	-3(1)
O(10)	44(1)	29(1)	36(1)	0(1)	-2(1)	1(1)
O(11)	33(1)	34(1)	24(1)	8(1)	-2(1)	0(1)

Table 69. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for s17phar9.

	x	y	z	U(eq)
H(3)	2215	3731	3770	32
H(4A)	969	2637	3483	38
H(5)	754	2138	2168	39
H(6A)	1729	2786	1128	42
H(7)	2964	3880	1402	37
H(8)	4143	6049	3523	28
H(10)	4187	4884	5743	30
H(11A)	1777	3881	5844	69
H(11B)	2786	4226	6346	69
H(11C)	2915	3403	5764	69
H(12A)	5179	6044	5533	31
H(12B)	4829	6819	4940	31
H(13)	6054	6455	4037	27
H(15)	7313	7043	4953	28
H(16A)	5955	7579	6590	47
H(16B)	6281	7860	5699	47
H(16C)	7186	7767	6375	47
H(17A)	8705	7079	5832	32
H(17B)	8507	6098	6122	32
H(18)	9383	6621	4625	33
H(20A)	10618	5101	4356	34
H(20B)	9822	4469	3870	34
H(21A)	10701	5965	2442	61
H(21B)	10665	4945	2641	61
H(21C)	11431	5577	3146	61

H(22A)	8858	3998	4983	32
H(22B)	9464	4568	5646	32
H(23A)	7853	3343	5924	36
H(23B)	6915	3841	6394	36
H(24A)	8239	3380	7301	68
H(24B)	8194	4422	7292	68
H(24C)	9130	3922	6822	68
H(25)	6239	4866	5608	26
H(26)	6854	3607	4683	27
H(27)	7019	4690	3384	30
H(28A)	8966	3433	2703	70
H(28B)	8769	4464	2687	70
H(28C)	7796	3810	2508	70
H(29)	7995	5873	3762	27
H(31)	5705	5235	3303	25
H(33A)	5704	1835	2787	70
H(33B)	6362	2675	2501	70
H(33C)	5086	2643	2393	70
H(34)	4109	3666	4501	28
H(4)	2530(30)	5776(19)	4897(18)	31(7)
H(6)	10320(40)	5840(30)	5830(30)	73(14)
H(11)	5260(30)	3020(20)	5300(20)	42(8)

Table 70. Torsion angles [°] for s17phar9.

O(1)-C(1)-C(2)-C(3)	178.4(2)
O(2)-C(1)-C(2)-C(3)	-2.5(3)
O(1)-C(1)-C(2)-C(7)	-3.7(4)
O(2)-C(1)-C(2)-C(7)	175.36(19)
C(7)-C(2)-C(3)-C(4)	0.7(3)
C(1)-C(2)-C(3)-C(4)	178.6(2)
C(2)-C(3)-C(4)-C(5)	0.6(3)
C(3)-C(4)-C(5)-C(6)	-1.6(4)
C(4)-C(5)-C(6)-C(7)	1.4(4)
C(5)-C(6)-C(7)-C(2)	-0.1(4)
C(3)-C(2)-C(7)-C(6)	-1.0(4)

C(1)-C(2)-C(7)-C(6)	-178.9(2)
O(2)-C(8)-C(9)-O(4)	-74.3(2)
C(31)-C(8)-C(9)-O(4)	163.63(17)
O(2)-C(8)-C(9)-C(12)	167.52(16)
C(31)-C(8)-C(9)-C(12)	45.4(2)
O(2)-C(8)-C(9)-C(10)	50.3(2)
C(31)-C(8)-C(9)-C(10)	-71.8(2)
O(4)-C(9)-C(10)-O(3)	32.5(2)
C(8)-C(9)-C(10)-O(3)	-93.72(19)
C(12)-C(9)-C(10)-O(3)	154.85(16)
O(4)-C(9)-C(10)-C(34)	153.93(17)
C(8)-C(9)-C(10)-C(34)	27.7(2)
C(12)-C(9)-C(10)-C(34)	-83.8(2)
O(4)-C(9)-C(12)-C(13)	-146.17(17)
C(8)-C(9)-C(12)-C(13)	-25.4(2)
C(10)-C(9)-C(12)-C(13)	91.2(2)
C(9)-C(12)-C(13)-C(31)	-3.4(2)
C(9)-C(12)-C(13)-C(14)	-132.07(18)
C(31)-C(13)-C(14)-C(25)	-51.2(2)
C(12)-C(13)-C(14)-C(25)	69.3(2)
C(31)-C(13)-C(14)-C(15)	-179.17(16)
C(12)-C(13)-C(14)-C(15)	-58.6(2)
C(31)-C(13)-C(14)-C(29)	57.1(2)
C(12)-C(13)-C(14)-C(29)	177.64(17)
C(25)-C(14)-C(15)-O(5)	-54.6(2)
C(29)-C(14)-C(15)-O(5)	-167.37(16)
C(13)-C(14)-C(15)-O(5)	67.9(2)
C(25)-C(14)-C(15)-C(17)	67.2(2)
C(29)-C(14)-C(15)-C(17)	-45.5(2)
C(13)-C(14)-C(15)-C(17)	-170.25(16)
O(5)-C(15)-C(17)-C(18)	167.80(18)
C(14)-C(15)-C(17)-C(18)	44.3(2)
C(15)-C(17)-C(18)-O(6)	-176.82(18)
C(15)-C(17)-C(18)-C(19)	-51.0(3)
O(6)-C(18)-C(19)-C(20)	-55.2(2)
C(17)-C(18)-C(19)-C(20)	-179.77(18)
O(6)-C(18)-C(19)-C(22)	64.2(2)
C(17)-C(18)-C(19)-C(22)	-60.4(2)
O(6)-C(18)-C(19)-C(29)	-175.80(17)

C(17)-C(18)-C(19)-C(29)	59.6(2)
C(22)-C(19)-C(20)-O(7)	168.78(17)
C(18)-C(19)-C(20)-O(7)	-70.1(2)
C(29)-C(19)-C(20)-O(7)	49.1(2)
C(20)-C(19)-C(22)-N	-167.08(17)
C(18)-C(19)-C(22)-N	75.4(2)
C(29)-C(19)-C(22)-N	-45.2(2)
C(15)-C(14)-C(25)-N	-51.8(2)
C(29)-C(14)-C(25)-N	67.91(18)
C(13)-C(14)-C(25)-N	-174.08(16)
C(15)-C(14)-C(25)-C(26)	-173.31(17)
C(29)-C(14)-C(25)-C(26)	-53.59(17)
C(13)-C(14)-C(25)-C(26)	64.42(18)
N-C(25)-C(26)-C(30)	163.45(16)
C(14)-C(25)-C(26)-C(30)	-77.38(19)
N-C(25)-C(26)-C(27)	-80.0(2)
C(14)-C(25)-C(26)-C(27)	39.15(19)
C(30)-C(26)-C(27)-O(8)	-121.50(18)
C(25)-C(26)-C(27)-O(8)	119.40(18)
C(30)-C(26)-C(27)-C(29)	110.18(18)
C(25)-C(26)-C(27)-C(29)	-8.9(2)
C(20)-C(19)-C(29)-C(27)	70.1(2)
C(22)-C(19)-C(29)-C(27)	-50.4(2)
C(18)-C(19)-C(29)-C(27)	-172.70(17)
C(20)-C(19)-C(29)-C(14)	-177.44(17)
C(22)-C(19)-C(29)-C(14)	62.1(2)
C(18)-C(19)-C(29)-C(14)	-60.2(2)
O(8)-C(27)-C(29)-C(19)	-29.3(2)
C(26)-C(27)-C(29)-C(19)	93.45(19)
O(8)-C(27)-C(29)-C(14)	-146.71(18)
C(26)-C(27)-C(29)-C(14)	-23.95(19)
C(25)-C(14)-C(29)-C(19)	-70.88(19)
C(15)-C(14)-C(29)-C(19)	53.2(2)
C(13)-C(14)-C(29)-C(19)	174.85(16)
C(25)-C(14)-C(29)-C(27)	48.17(17)
C(15)-C(14)-C(29)-C(27)	172.22(16)
C(13)-C(14)-C(29)-C(27)	-66.10(19)
C(27)-C(26)-C(30)-O(9)	60.8(2)
C(25)-C(26)-C(30)-O(9)	175.28(15)

C(27)-C(26)-C(30)-C(31)	-48.1(2)
C(25)-C(26)-C(30)-C(31)	66.3(2)
C(27)-C(26)-C(30)-C(34)	-177.48(17)
C(25)-C(26)-C(30)-C(34)	-63.0(2)
O(2)-C(8)-C(31)-C(30)	-45.7(2)
C(9)-C(8)-C(31)-C(30)	71.8(2)
O(2)-C(8)-C(31)-C(13)	-165.84(16)
C(9)-C(8)-C(31)-C(13)	-48.35(19)
O(9)-C(30)-C(31)-C(8)	90.60(18)
C(26)-C(30)-C(31)-C(8)	-156.71(16)
C(34)-C(30)-C(31)-C(8)	-25.8(2)
O(9)-C(30)-C(31)-C(13)	-154.95(16)
C(26)-C(30)-C(31)-C(13)	-42.3(2)
C(34)-C(30)-C(31)-C(13)	88.6(2)
C(14)-C(13)-C(31)-C(8)	158.31(16)
C(12)-C(13)-C(31)-C(8)	31.18(19)
C(14)-C(13)-C(31)-C(30)	38.0(2)
C(12)-C(13)-C(31)-C(30)	-89.08(19)
O(3)-C(10)-C(34)-O(11)	-93.27(19)
C(9)-C(10)-C(34)-O(11)	146.96(17)
O(3)-C(10)-C(34)-C(30)	138.86(17)
C(9)-C(10)-C(34)-C(30)	19.1(3)
O(9)-C(30)-C(34)-O(11)	102.42(19)
C(26)-C(30)-C(34)-O(11)	-18.5(2)
C(31)-C(30)-C(34)-O(11)	-145.30(17)
O(9)-C(30)-C(34)-C(10)	-132.45(18)
C(26)-C(30)-C(34)-C(10)	106.6(2)
C(31)-C(30)-C(34)-C(10)	-20.2(2)
C(14)-C(25)-N-C(23)	172.79(17)
C(26)-C(25)-N-C(23)	-74.6(2)
C(14)-C(25)-N-C(22)	-59.3(2)
C(26)-C(25)-N-C(22)	53.3(2)
C(24)-C(23)-N-C(25)	-152.3(2)
C(24)-C(23)-N-C(22)	77.4(3)
C(19)-C(22)-N-C(25)	45.0(2)
C(19)-C(22)-N-C(23)	173.64(17)
O(1)-C(1)-O(2)-C(8)	-4.4(3)
C(2)-C(1)-O(2)-C(8)	176.52(17)
C(31)-C(8)-O(2)-C(1)	-69.3(2)

C(9)-C(8)-O(2)-C(1)	177.01(17)
C(34)-C(10)-O(3)-C(11)	79.4(2)
C(9)-C(10)-O(3)-C(11)	-155.5(2)
C(17)-C(15)-O(5)-C(16)	85.8(2)
C(14)-C(15)-O(5)-C(16)	-147.41(18)
C(19)-C(20)-O(7)-C(21)	178.2(2)
C(26)-C(27)-O(8)-C(28)	144.9(2)
C(29)-C(27)-O(8)-C(28)	-94.9(2)
O(10)-C(32)-O(9)-C(30)	11.7(3)
C(33)-C(32)-O(9)-C(30)	-167.6(2)
C(26)-C(30)-O(9)-C(32)	66.5(2)
C(31)-C(30)-O(9)-C(32)	179.99(18)
C(34)-C(30)-O(9)-C(32)	-60.0(2)

Table 71. Hydrogen bonds for s17phar9 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(4)-H(4)...O(3)	0.87(3)	2.01(3)	2.569(2)	121(3)

s17phar8: lycoctonine monohydrate (**3d**)

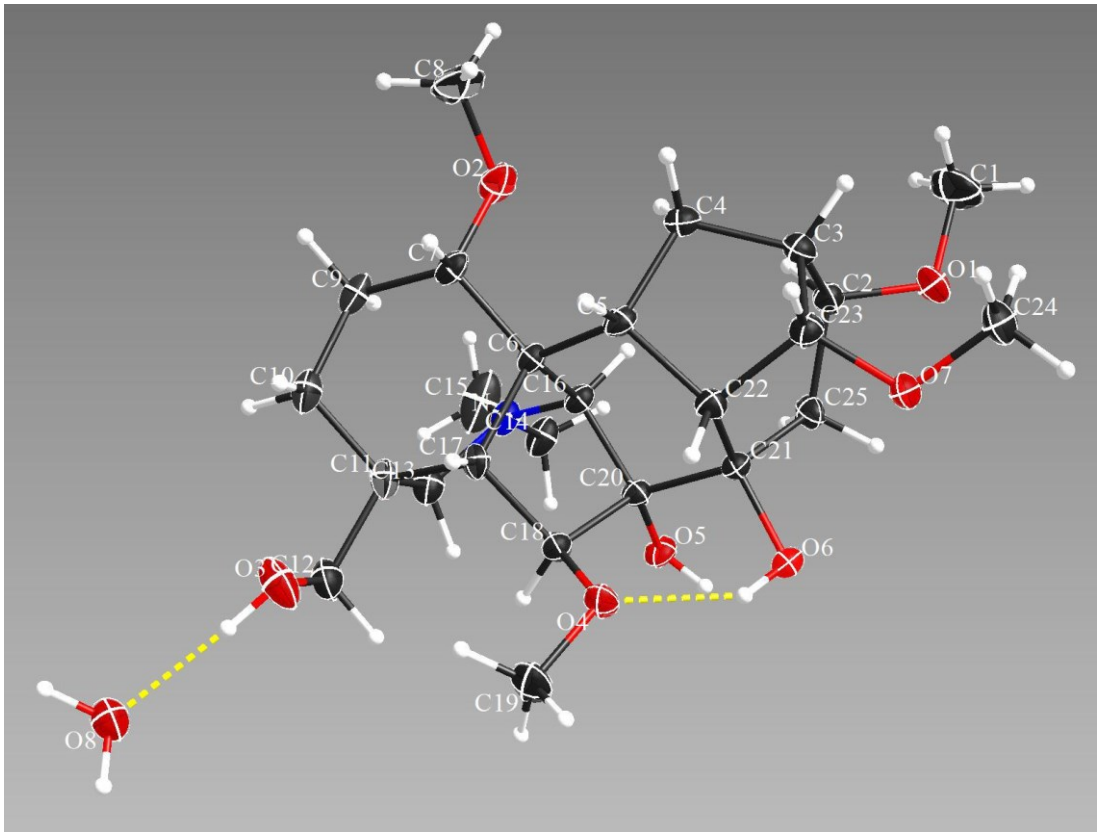

Table 72. Crystal data and structure refinement for s17phar8.

Identification code	s17phar8	
Empirical formula	C25 H43 N O8	
Formula weight	485.60	
Temperature	150.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 11.1092(2) Å	α= 90°.
	b = 7.81270(10) Å	β= 104.010(2)°.
	c = 14.7090(3) Å	γ = 90°.
Volume	1238.66(4) $Å^3$	
Z	2	
Density (calculated)	1.302 Mg/m^3	
Absorption coefficient	0.788 mm^{-1}	
F(000)	528	
Crystal size	0.230 x 0.120 x 0.050 mm^3	

Theta range for data collection	3.097 to 73.179°.
Index ranges	-13<=h<=13, -6<=k<=9, -18<=l<=18
Reflections collected	10105
Independent reflections	3845 [R(int) = 0.0295]
Completeness to theta = 1.000°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.93589
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3845 / 1 / 332
Goodness-of-fit on F^2	1.037
Final R indices [I>2sigma(I)]	R1 = 0.0311, wR2 = 0.0771
R indices (all data)	R1 = 0.0330, wR2 = 0.0787
Absolute structure parameter	0.13(13)
Extinction coefficient	n/a
Largest diff. peak and hole	0.203 and -0.185 e.$Å^{-3}$

Table 73. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for s17phar8. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	12635(2)	8558(4)	3151(2)	43(1)
C(2)	10566(2)	7486(3)	2589(1)	19(1)
C(3)	10774(2)	5664(3)	2257(1)	20(1)
C(4)	10171(2)	4328(3)	2770(2)	21(1)
C(5)	8812(2)	4056(2)	2166(1)	16(1)
C(6)	7774(2)	4171(2)	2718(1)	15(1)
C(7)	8028(2)	2750(2)	3482(1)	18(1)
C(8)	9793(3)	1575(4)	4531(2)	44(1)
C(9)	7006(2)	2411(3)	3989(1)	22(1)
C(10)	5762(2)	2235(3)	3296(2)	23(1)
C(11)	5479(2)	3827(3)	2676(1)	20(1)
C(12)	4140(2)	3670(3)	2084(2)	25(1)
C(13)	5550(2)	5483(3)	3267(2)	22(1)
C(14)	6788(2)	7790(3)	4105(2)	23(1)
C(15)	6545(3)	7610(4)	5072(2)	47(1)
C(16)	7656(2)	6030(2)	3023(1)	16(1)

C(17)	6434(2)	3973(2)	2063(1)	16(1)
C(18)	6194(2)	5682(3)	1516(1)	16(1)
C(19)	5011(2)	4879(3)	3(2)	31(1)
C(20)	7218(2)	6922(2)	2052(1)	15(1)
C(21)	8282(2)	7113(2)	1543(1)	15(1)
C(22)	8723(2)	5322(2)	1336(1)	16(1)
C(23)	10066(2)	5357(3)	1243(1)	18(1)
C(24)	11452(2)	6534(3)	413(2)	26(1)
C(25)	9333(2)	8295(3)	2072(1)	19(1)
N	6811(2)	6135(2)	3645(1)	19(1)
O(1)	11502(1)	8662(2)	2452(1)	26(1)
O(2)	9151(2)	3083(2)	4174(1)	28(1)
O(3)	4012(2)	2181(2)	1517(1)	32(1)
O(4)	6157(1)	5538(2)	538(1)	21(1)
O(5)	6726(1)	8573(2)	2162(1)	19(1)
O(6)	7773(1)	8044(2)	688(1)	19(1)
O(7)	10228(1)	6588(2)	565(1)	21(1)
O(8)	1579(2)	1323(3)	1176(1)	35(1)

Table 74. Bond lengths [Å] for s17phar8.

C(1)-O(1)	1.422(3)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(2)-O(1)	1.438(2)
C(2)-C(25)	1.533(3)
C(2)-C(3)	1.541(3)
C(2)-H(2)	1.0000
C(3)-C(23)	1.527(3)
C(3)-C(4)	1.533(3)
C(3)-H(3A)	1.0000
C(4)-C(5)	1.570(3)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(22)	1.556(3)

C(5)-C(6)	1.565(2)
C(5)-H(5A)	1.0000
C(6)-C(16)	1.535(2)
C(6)-C(7)	1.557(3)
C(6)-C(17)	1.572(3)
C(7)-O(2)	1.430(2)
C(7)-C(9)	1.523(3)
C(7)-H(7)	1.0000
C(8)-O(2)	1.411(3)
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-C(10)	1.512(3)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(11)	1.529(3)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.536(3)
C(11)-C(13)	1.550(3)
C(11)-C(17)	1.554(2)
C(12)-O(3)	1.418(3)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-N	1.468(3)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-N	1.462(3)
C(14)-C(15)	1.517(3)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-N	1.463(2)
C(16)-C(20)	1.558(3)
C(16)-H(16)	1.0000
C(17)-C(18)	1.549(3)
C(17)-H(17)	1.0000

C(18)-O(4)	1.433(2)
C(18)-C(20)	1.554(3)
C(18)-H(18)	1.0000
C(19)-O(4)	1.422(3)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-O(5)	1.425(2)
C(20)-C(21)	1.552(2)
C(21)-O(6)	1.445(2)
C(21)-C(22)	1.536(3)
C(21)-C(25)	1.543(3)
C(22)-C(23)	1.532(2)
C(22)-H(22)	1.0000
C(23)-O(7)	1.427(2)
C(23)-H(23)	1.0000
C(24)-O(7)	1.431(2)
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
O(3)-H(3)	0.85(3)
O(5)-H(5)	0.81(3)
O(6)-H(6)	0.88(3)
O(8)-H(8D)	0.87(4)
O(8)-H(8E)	0.88(5)

Table 75. Bond angles [°] for s17phar8.

O(1)-C(1)-H(1A)	109.5
O(1)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
O(1)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5

O(1)-C(2)-C(25)	104.86(16)
O(1)-C(2)-C(3)	112.12(16)
C(25)-C(2)-C(3)	114.06(16)
O(1)-C(2)-H(2)	108.5
C(25)-C(2)-H(2)	108.5
C(3)-C(2)-H(2)	108.5
C(23)-C(3)-C(4)	101.01(16)
C(23)-C(3)-C(2)	111.96(16)
C(4)-C(3)-C(2)	110.84(16)
C(23)-C(3)-H(3A)	110.9
C(4)-C(3)-H(3A)	110.9
C(2)-C(3)-H(3A)	110.9
C(3)-C(4)-C(5)	106.79(15)
C(3)-C(4)-H(4A)	110.4
C(5)-C(4)-H(4A)	110.4
C(3)-C(4)-H(4B)	110.4
C(5)-C(4)-H(4B)	110.4
H(4A)-C(4)-H(4B)	108.6
C(22)-C(5)-C(6)	117.07(15)
C(22)-C(5)-C(4)	103.12(15)
C(6)-C(5)-C(4)	115.33(15)
C(22)-C(5)-H(5A)	106.9
C(6)-C(5)-H(5A)	106.9
C(4)-C(5)-H(5A)	106.9
C(16)-C(6)-C(7)	118.46(15)
C(16)-C(6)-C(5)	109.41(15)
C(7)-C(6)-C(5)	107.81(15)
C(16)-C(6)-C(17)	97.91(14)
C(7)-C(6)-C(17)	110.54(15)
C(5)-C(6)-C(17)	112.58(15)
O(2)-C(7)-C(9)	107.99(16)
O(2)-C(7)-C(6)	110.99(15)
C(9)-C(7)-C(6)	116.81(16)
O(2)-C(7)-H(7)	106.8
C(9)-C(7)-H(7)	106.8
C(6)-C(7)-H(7)	106.8
O(2)-C(8)-H(8A)	109.5
O(2)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5

O(2)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(10)-C(9)-C(7)	110.74(16)
C(10)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9A)	109.5
C(10)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	108.1
C(9)-C(10)-C(11)	110.54(18)
C(9)-C(10)-H(10A)	109.5
C(11)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10B)	109.5
C(11)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	108.1
C(10)-C(11)-C(12)	107.73(17)
C(10)-C(11)-C(13)	111.67(17)
C(12)-C(11)-C(13)	107.16(17)
C(10)-C(11)-C(17)	109.56(16)
C(12)-C(11)-C(17)	112.41(17)
C(13)-C(11)-C(17)	108.33(16)
O(3)-C(12)-C(11)	110.13(17)
O(3)-C(12)-H(12A)	109.6
C(11)-C(12)-H(12A)	109.6
O(3)-C(12)-H(12B)	109.6
C(11)-C(12)-H(12B)	109.6
H(12A)-C(12)-H(12B)	108.1
N-C(13)-C(11)	114.63(16)
N-C(13)-H(13A)	108.6
C(11)-C(13)-H(13A)	108.6
N-C(13)-H(13B)	108.6
C(11)-C(13)-H(13B)	108.6
H(13A)-C(13)-H(13B)	107.6
N-C(14)-C(15)	112.26(18)
N-C(14)-H(14A)	109.2
C(15)-C(14)-H(14A)	109.2
N-C(14)-H(14B)	109.2
C(15)-C(14)-H(14B)	109.2
H(14A)-C(14)-H(14B)	107.9

C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
N-C(16)-C(6)	110.43(15)
N-C(16)-C(20)	116.30(15)
C(6)-C(16)-C(20)	100.59(14)
N-C(16)-H(16)	109.7
C(6)-C(16)-H(16)	109.7
C(20)-C(16)-H(16)	109.7
C(18)-C(17)-C(11)	107.98(16)
C(18)-C(17)-C(6)	104.55(15)
C(11)-C(17)-C(6)	109.29(15)
C(18)-C(17)-H(17)	111.6
C(11)-C(17)-H(17)	111.6
C(6)-C(17)-H(17)	111.6
O(4)-C(18)-C(17)	114.41(16)
O(4)-C(18)-C(20)	113.40(15)
C(17)-C(18)-C(20)	105.15(15)
O(4)-C(18)-H(18)	107.9
C(17)-C(18)-H(18)	107.9
C(20)-C(18)-H(18)	107.9
O(4)-C(19)-H(19A)	109.5
O(4)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
O(4)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
O(5)-C(20)-C(21)	109.00(15)
O(5)-C(20)-C(18)	111.60(15)
C(21)-C(20)-C(18)	111.41(15)
O(5)-C(20)-C(16)	110.06(15)
C(21)-C(20)-C(16)	112.32(15)
C(18)-C(20)-C(16)	102.35(15)
O(6)-C(21)-C(22)	111.25(15)
O(6)-C(21)-C(25)	103.04(16)
C(22)-C(21)-C(25)	114.00(16)

O(6)-C(21)-C(20)	106.56(14)
C(22)-C(21)-C(20)	108.93(15)
C(25)-C(21)-C(20)	112.72(15)
C(23)-C(22)-C(21)	111.43(16)
C(23)-C(22)-C(5)	101.73(15)
C(21)-C(22)-C(5)	112.73(15)
C(23)-C(22)-H(22)	110.2
C(21)-C(22)-H(22)	110.2
C(5)-C(22)-H(22)	110.2
O(7)-C(23)-C(3)	117.02(17)
O(7)-C(23)-C(22)	111.38(16)
C(3)-C(23)-C(22)	101.41(15)
O(7)-C(23)-H(23)	108.9
C(3)-C(23)-H(23)	108.9
C(22)-C(23)-H(23)	108.9
O(7)-C(24)-H(24A)	109.5
O(7)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
O(7)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(2)-C(25)-C(21)	118.62(17)
C(2)-C(25)-H(25A)	107.7
C(21)-C(25)-H(25A)	107.7
C(2)-C(25)-H(25B)	107.7
C(21)-C(25)-H(25B)	107.7
H(25A)-C(25)-H(25B)	107.1
C(14)-N-C(16)	115.11(16)
C(14)-N-C(13)	111.13(17)
C(16)-N-C(13)	116.22(15)
C(1)-O(1)-C(2)	113.96(18)
C(8)-O(2)-C(7)	112.87(17)
C(12)-O(3)-H(3)	107(2)
C(19)-O(4)-C(18)	112.89(16)
C(20)-O(5)-H(5)	105(2)
C(21)-O(6)-H(6)	103(2)
C(23)-O(7)-C(24)	111.97(16)
H(8D)-O(8)-H(8E)	109(3)

Table 76. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for s17phar8. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	23(1)	44(2)	54(2)	-3(1)	-8(1)	-6(1)
C(2)	17(1)	21(1)	19(1)	0(1)	4(1)	-2(1)
C(3)	15(1)	22(1)	22(1)	2(1)	5(1)	3(1)
C(4)	18(1)	21(1)	24(1)	6(1)	4(1)	4(1)
C(5)	19(1)	13(1)	17(1)	1(1)	6(1)	4(1)
C(6)	17(1)	12(1)	15(1)	0(1)	4(1)	0(1)
C(7)	25(1)	11(1)	17(1)	-1(1)	4(1)	0(1)
C(8)	40(1)	42(2)	37(1)	18(1)	-13(1)	1(1)
C(9)	35(1)	13(1)	21(1)	2(1)	13(1)	0(1)
C(10)	28(1)	17(1)	28(1)	1(1)	16(1)	-2(1)
C(11)	22(1)	15(1)	25(1)	-2(1)	11(1)	-2(1)
C(12)	21(1)	22(1)	34(1)	-1(1)	11(1)	-3(1)
C(13)	25(1)	16(1)	27(1)	-1(1)	13(1)	1(1)
C(14)	36(1)	14(1)	24(1)	-2(1)	15(1)	2(1)
C(15)	87(2)	29(1)	38(1)	-11(1)	39(2)	-8(1)
C(16)	19(1)	12(1)	16(1)	-1(1)	4(1)	1(1)
C(17)	18(1)	13(1)	19(1)	-2(1)	6(1)	-2(1)
C(18)	15(1)	17(1)	17(1)	0(1)	4(1)	-1(1)
C(19)	26(1)	38(1)	24(1)	0(1)	-3(1)	-13(1)
C(20)	15(1)	12(1)	18(1)	0(1)	4(1)	2(1)
C(21)	15(1)	14(1)	16(1)	2(1)	4(1)	1(1)
C(22)	17(1)	16(1)	16(1)	0(1)	4(1)	1(1)
C(23)	19(1)	16(1)	20(1)	1(1)	7(1)	2(1)
C(24)	21(1)	32(1)	29(1)	3(1)	13(1)	2(1)
C(25)	16(1)	14(1)	27(1)	0(1)	5(1)	-2(1)
N	27(1)	12(1)	20(1)	-2(1)	11(1)	0(1)
O(1)	17(1)	29(1)	30(1)	0(1)	0(1)	-7(1)
O(2)	33(1)	27(1)	18(1)	5(1)	-3(1)	-8(1)
O(3)	24(1)	30(1)	44(1)	-12(1)	10(1)	-9(1)
O(4)	18(1)	27(1)	16(1)	0(1)	0(1)	-6(1)
O(5)	22(1)	12(1)	24(1)	2(1)	8(1)	5(1)
O(6)	20(1)	18(1)	18(1)	5(1)	3(1)	1(1)
O(7)	18(1)	25(1)	23(1)	5(1)	9(1)	3(1)
O(8)	30(1)	36(1)	35(1)	7(1)	0(1)	-12(1)

Table 77. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for s17phar8.

	x	y	z	U(eq)
H(1A)	13225	9396	3016	65
H(1B)	12982	7404	3153	65
H(1C)	12480	8802	3767	65
H(2)	10591	7442	3273	23
H(3A)	11678	5425	2342	24
H(4A)	10161	4741	3404	25
H(4B)	10640	3240	2832	25
H(5A)	8774	2874	1899	19
H(7)	8156	1659	3163	21
H(8A)	10557	1876	4995	66
H(8B)	10001	932	4018	66
H(8C)	9268	870	4829	66
H(9A)	7195	1347	4361	27
H(9B)	6974	3366	4424	27
H(10A)	5105	2078	3639	28
H(10B)	5768	1213	2900	28
H(12A)	3563	3607	2502	30
H(12B)	3924	4694	1682	30
H(13A)	5055	6384	2872	26
H(13B)	5164	5258	3795	26
H(14A)	6134	8514	3711	28
H(14B)	7594	8372	4160	28
H(15A)	6601	8736	5372	71
H(15B)	7162	6840	5452	71
H(15C)	5712	7137	5015	71
H(16)	8491	6476	3354	19
H(17)	6381	2972	1631	20
H(18)	5374	6135	1574	20
H(19A)	5052	4749	-651	46
H(19B)	4339	5671	38	46
H(19C)	4852	3762	254	46
H(22)	8164	4848	753	20
H(23)	10287	4199	1044	22

H(24A)	11475	7209	-144	39
H(24B)	11676	5345	320	39
H(24C)	12042	7011	960	39
H(25A)	9514	9126	1614	23
H(25B)	9009	8958	2535	23
H(3)	3250(30)	1910(50)	1370(20)	46(9)
H(5)	6760(30)	9090(40)	1690(20)	32(8)
H(6)	7190(30)	7350(40)	380(20)	39(8)
H(8D)	1040(30)	1400(50)	630(30)	55(11)
H(8E)	1430(40)	390(60)	1470(30)	73(13)

Table 78. Torsion angles [°] for s17phar8.

O(1)-C(2)-C(3)-C(23)	-92.75(19)
C(25)-C(2)-C(3)-C(23)	26.2(2)
O(1)-C(2)-C(3)-C(4)	155.29(16)
C(25)-C(2)-C(3)-C(4)	-85.7(2)
C(23)-C(3)-C(4)-C(5)	-28.51(19)
C(2)-C(3)-C(4)-C(5)	90.29(19)
C(3)-C(4)-C(5)-C(22)	-1.2(2)
C(3)-C(4)-C(5)-C(6)	-130.01(17)
C(22)-C(5)-C(6)-C(16)	-52.0(2)
C(4)-C(5)-C(6)-C(16)	69.6(2)
C(22)-C(5)-C(6)-C(7)	177.89(16)
C(4)-C(5)-C(6)-C(7)	-60.5(2)
C(22)-C(5)-C(6)-C(17)	55.7(2)
C(4)-C(5)-C(6)-C(17)	177.30(16)
C(16)-C(6)-C(7)-O(2)	-58.4(2)
C(5)-C(6)-C(7)-O(2)	66.39(19)
C(17)-C(6)-C(7)-O(2)	-170.18(15)
C(16)-C(6)-C(7)-C(9)	65.9(2)
C(5)-C(6)-C(7)-C(9)	-169.24(16)
C(17)-C(6)-C(7)-C(9)	-45.8(2)
O(2)-C(7)-C(9)-C(10)	173.94(16)
C(6)-C(7)-C(9)-C(10)	48.1(2)
C(7)-C(9)-C(10)-C(11)	-56.2(2)

C(9)-C(10)-C(11)-C(12)	-172.58(16)
C(9)-C(10)-C(11)-C(13)	-55.2(2)
C(9)-C(10)-C(11)-C(17)	64.9(2)
C(10)-C(11)-C(12)-O(3)	-60.2(2)
C(13)-C(11)-C(12)-O(3)	179.47(16)
C(17)-C(11)-C(12)-O(3)	60.6(2)
C(10)-C(11)-C(13)-N	80.6(2)
C(12)-C(11)-C(13)-N	-161.62(17)
C(17)-C(11)-C(13)-N	-40.1(2)
C(7)-C(6)-C(16)-N	-48.4(2)
C(5)-C(6)-C(16)-N	-172.49(14)
C(17)-C(6)-C(16)-N	70.13(18)
C(7)-C(6)-C(16)-C(20)	-171.86(16)
C(5)-C(6)-C(16)-C(20)	64.10(18)
C(17)-C(6)-C(16)-C(20)	-53.29(16)
C(10)-C(11)-C(17)-C(18)	-174.75(17)
C(12)-C(11)-C(17)-C(18)	65.5(2)
C(13)-C(11)-C(17)-C(18)	-52.7(2)
C(10)-C(11)-C(17)-C(6)	-61.6(2)
C(12)-C(11)-C(17)-C(6)	178.68(17)
C(13)-C(11)-C(17)-C(6)	60.5(2)
C(16)-C(6)-C(17)-C(18)	41.82(17)
C(7)-C(6)-C(17)-C(18)	166.29(15)
C(5)-C(6)-C(17)-C(18)	-73.08(18)
C(16)-C(6)-C(17)-C(11)	-73.57(17)
C(7)-C(6)-C(17)-C(11)	50.9(2)
C(5)-C(6)-C(17)-C(11)	171.53(15)
C(11)-C(17)-C(18)-O(4)	-132.98(16)
C(6)-C(17)-C(18)-O(4)	110.72(17)
C(11)-C(17)-C(18)-C(20)	101.94(17)
C(6)-C(17)-C(18)-C(20)	-14.36(18)
O(4)-C(18)-C(20)-O(5)	98.10(19)
C(17)-C(18)-C(20)-O(5)	-136.19(16)
O(4)-C(18)-C(20)-C(21)	-24.0(2)
C(17)-C(18)-C(20)-C(21)	101.72(16)
O(4)-C(18)-C(20)-C(16)	-144.22(16)
C(17)-C(18)-C(20)-C(16)	-18.52(18)
N-C(16)-C(20)-O(5)	45.0(2)
C(6)-C(16)-C(20)-O(5)	164.24(15)

N-C(16)-C(20)-C(21)	166.64(15)
C(6)-C(16)-C(20)-C(21)	-74.11(18)
N-C(16)-C(20)-C(18)	-73.76(19)
C(6)-C(16)-C(20)-C(18)	45.49(17)
O(5)-C(20)-C(21)-O(6)	-54.25(19)
C(18)-C(20)-C(21)-O(6)	69.33(19)
C(16)-C(20)-C(21)-O(6)	-176.51(15)
O(5)-C(20)-C(21)-C(22)	-174.37(15)
C(18)-C(20)-C(21)-C(22)	-50.8(2)
C(16)-C(20)-C(21)-C(22)	63.38(19)
O(5)-C(20)-C(21)-C(25)	58.1(2)
C(18)-C(20)-C(21)-C(25)	-178.36(16)
C(16)-C(20)-C(21)-C(25)	-64.2(2)
O(6)-C(21)-C(22)-C(23)	87.69(19)
C(25)-C(21)-C(22)-C(23)	-28.3(2)
C(20)-C(21)-C(22)-C(23)	-155.14(15)
O(6)-C(21)-C(22)-C(5)	-158.66(15)
C(25)-C(21)-C(22)-C(5)	85.35(19)
C(20)-C(21)-C(22)-C(5)	-41.5(2)
C(6)-C(5)-C(22)-C(23)	158.12(16)
C(4)-C(5)-C(22)-C(23)	30.35(18)
C(6)-C(5)-C(22)-C(21)	38.7(2)
C(4)-C(5)-C(22)-C(21)	-89.09(18)
C(4)-C(3)-C(23)-O(7)	169.29(16)
C(2)-C(3)-C(23)-O(7)	51.3(2)
C(4)-C(3)-C(23)-C(22)	47.93(18)
C(2)-C(3)-C(23)-C(22)	-70.06(19)
C(21)-C(22)-C(23)-O(7)	-54.1(2)
C(5)-C(22)-C(23)-O(7)	-174.46(15)
C(21)-C(22)-C(23)-C(3)	71.11(19)
C(5)-C(22)-C(23)-C(3)	-49.24(18)
O(1)-C(2)-C(25)-C(21)	142.54(17)
C(3)-C(2)-C(25)-C(21)	19.5(2)
O(6)-C(21)-C(25)-C(2)	-139.08(17)
C(22)-C(21)-C(25)-C(2)	-18.4(2)
C(20)-C(21)-C(25)-C(2)	106.5(2)
C(15)-C(14)-N-C(16)	-147.5(2)
C(15)-C(14)-N-C(13)	77.7(3)
C(6)-C(16)-N-C(14)	170.15(16)

C(20)-C(16)-N-C(14)	-76.1(2)
C(6)-C(16)-N-C(13)	-57.4(2)
C(20)-C(16)-N-C(13)	56.3(2)
C(11)-C(13)-N-C(14)	173.87(16)
C(11)-C(13)-N-C(16)	39.7(2)
C(25)-C(2)-O(1)-C(1)	156.0(2)
C(3)-C(2)-O(1)-C(1)	-79.8(2)
C(9)-C(7)-O(2)-C(8)	84.9(2)
C(6)-C(7)-O(2)-C(8)	-145.9(2)
C(17)-C(18)-O(4)-C(19)	78.5(2)
C(20)-C(18)-O(4)-C(19)	-160.90(18)
C(3)-C(23)-O(7)-C(24)	69.0(2)
C(22)-C(23)-O(7)-C(24)	-175.06(17)

Table 79. Hydrogen bonds for s17phar8 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(3)-H(3)...O(8)	0.85(3)	1.87(3)	2.710(2)	175(3)
O(5)-H(5)...O(6)	0.81(3)	2.22(3)	2.729(2)	121(3)
O(6)-H(6)...O(4)	0.88(3)	1.87(3)	2.630(2)	143(3)
O(8)-H(8D)...O(7)#1	0.87(4)	1.98(4)	2.853(2)	178(3)
O(8)-H(8E)...O(1)#2	0.88(5)	1.97(5)	2.817(2)	161(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y-1/2,-z #2 x-1,y-1,z

s17phar13: lappaconitine monohydrate (**27b**)

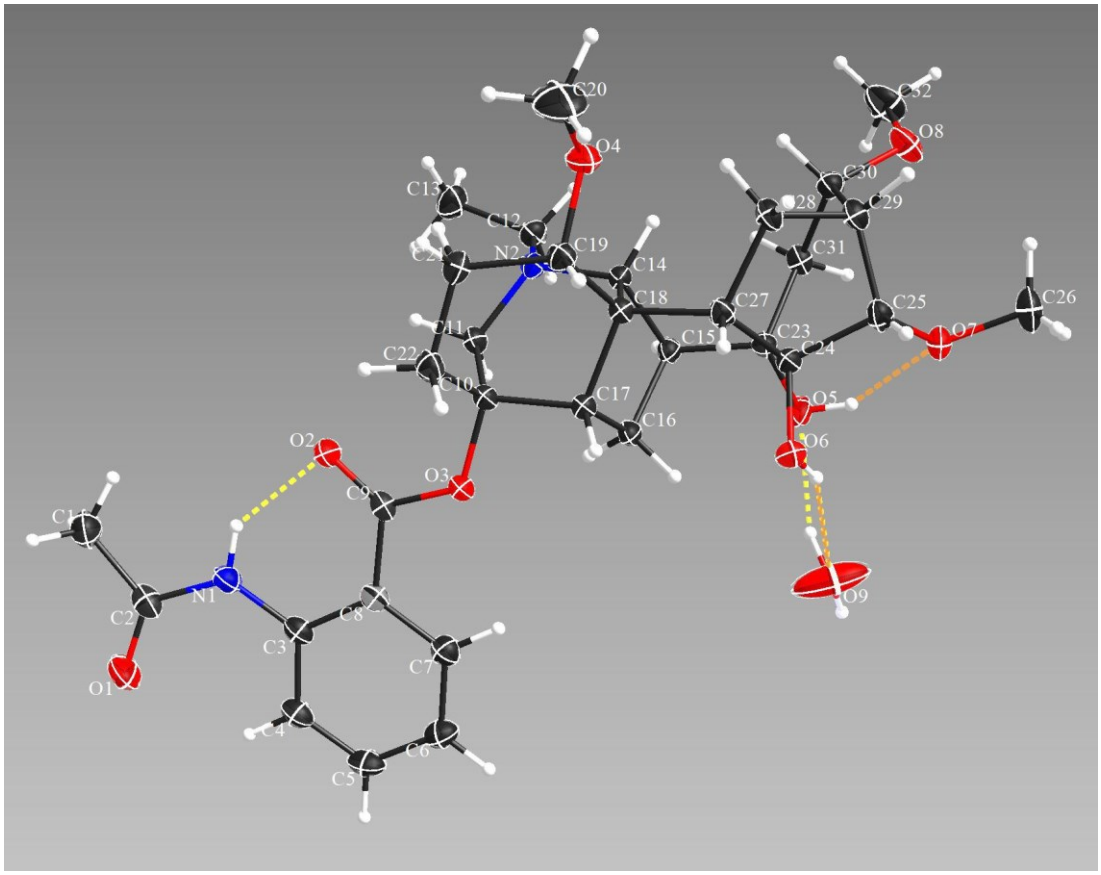

Table 80. Crystal data and structure refinement for s17phar13.

Identification code	s17phar13	
Empirical formula	C32 H44.50 N2 O8.25	
Formula weight	589.19	
Temperature	150.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Trigonal	
Space group	$P3_121$	
Unit cell dimensions	a = 10.7396(2) Å	α= 90°.
	b = 10.7396(2) Å	β= 90°.
	c = 43.9565(9) Å	γ = 120°.
Volume	4390.66(19) $Å^3$	
Z	6	
Density (calculated)	1.337 Mg/m^3	
Absorption coefficient	0.787 mm^{-1}	
F(000)	1899	

Crystal size	0.200 x 0.200 x 0.080 mm^3
Theta range for data collection	3.016 to 73.129°.
Index ranges	-13<=h<=12, -13<=k<=13, -54<=l<=52
Reflections collected	44047
Independent reflections	5853 [R(int) = 0.0340]
Completeness to theta = 67.684°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.80203
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5853 / 1 / 405
Goodness-of-fit on F^2	1.120
Final R indices [I>2sigma(I)]	R1 = 0.0332, wR2 = 0.0849
R indices (all data)	R1 = 0.0336, wR2 = 0.0852
Absolute structure parameter	-0.04(4)
Extinction coefficient	n/a
Largest diff. peak and hole	0.230 and -0.173 e.$Å^{-3}$

Table 81. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for s17phar13. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	8882(3)	11490(3)	2096(1)	33(1)
C(2)	7868(3)	9983(3)	1988(1)	26(1)
C(3)	6313(2)	7501(2)	2192(1)	20(1)
C(4)	5997(2)	6780(3)	1912(1)	25(1)
C(5)	5019(3)	5333(3)	1894(1)	28(1)
C(6)	4327(3)	4540(2)	2151(1)	28(1)
C(7)	4657(2)	5222(2)	2431(1)	24(1)
C(8)	5647(2)	6690(2)	2458(1)	20(1)
C(9)	5990(2)	7366(2)	2766(1)	20(1)
C(10)	5292(2)	6868(2)	3304(1)	19(1)
C(11)	6833(2)	7379(2)	3418(1)	19(1)
C(12)	8303(2)	7318(2)	3826(1)	21(1)
C(13)	9557(2)	8816(3)	3763(1)	29(1)
C(14)	5715(2)	5862(2)	3881(1)	15(1)
C(15)	5475(2)	4427(2)	3740(1)	17(1)

C(16)	4775(2)	4379(2)	3429(1)	19(1)
C(17)	4223(2)	5457(2)	3462(1)	17(1)
C(18)	4271(2)	5763(2)	3812(1)	16(1)
C(19)	4115(2)	7107(2)	3876(1)	19(1)
C(20)	3942(4)	8381(4)	4302(1)	51(1)
C(21)	4941(2)	8405(2)	3669(1)	21(1)
C(22)	4821(2)	7975(2)	3337(1)	22(1)
C(23)	4478(2)	3146(2)	3940(1)	17(1)
C(24)	2952(2)	2992(2)	3957(1)	18(1)
C(25)	2219(2)	2206(2)	4250(1)	20(1)
C(26)	1542(3)	57(3)	4524(1)	32(1)
C(27)	3035(2)	4461(2)	3988(1)	17(1)
C(28)	3022(2)	4655(2)	4341(1)	20(1)
C(29)	3022(2)	3354(2)	4490(1)	19(1)
C(30)	4561(2)	3657(2)	4536(1)	19(1)
C(31)	5169(2)	3258(2)	4257(1)	19(1)
C(32)	5965(3)	3262(3)	4894(1)	36(1)
N(1)	7279(2)	8978(2)	2217(1)	23(1)
N(2)	6912(2)	7171(2)	3749(1)	17(1)
O(1)	7611(2)	9708(2)	1719(1)	42(1)
O(2)	6907(2)	8601(2)	2817(1)	26(1)
O(3)	5164(2)	6431(2)	2981(1)	21(1)
O(4)	4534(2)	7572(2)	4184(1)	28(1)
O(5)	4336(2)	1880(2)	3792(1)	23(1)
O(6)	2093(2)	2267(2)	3698(1)	24(1)
O(7)	2297(2)	922(2)	4270(1)	23(1)
O(8)	4552(2)	2842(2)	4795(1)	27(1)
O(9)	2713(6)	0	3333	74(3)

Table 82. Bond lengths [Å] for s17phar13.

C(1)-C(2)	1.506(3)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(2)-O(1)	1.216(3)

C(2)-N(1)	1.376(3)
C(3)-N(1)	1.400(3)
C(3)-C(4)	1.406(3)
C(3)-C(8)	1.419(3)
C(4)-C(5)	1.375(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.385(3)
C(5)-H(5)	0.9500
C(6)-C(7)	1.387(3)
C(6)-H(6)	0.9500
C(7)-C(8)	1.398(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.493(3)
C(9)-O(2)	1.214(3)
C(9)-O(3)	1.339(2)
C(10)-O(3)	1.481(2)
C(10)-C(22)	1.513(3)
C(10)-C(17)	1.535(3)
C(10)-C(11)	1.542(3)
C(11)-N(2)	1.482(2)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-N(2)	1.462(3)
C(12)-C(13)	1.520(3)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-N(2)	1.470(2)
C(14)-C(18)	1.531(3)
C(14)-C(15)	1.559(3)
C(14)-H(14)	1.0000
C(15)-C(23)	1.528(3)
C(15)-C(16)	1.547(3)
C(15)-H(15)	1.0000
C(16)-C(17)	1.548(3)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900

C(17)-C(18)	1.567(2)
C(17)-H(17)	1.0000
C(18)-C(19)	1.560(3)
C(18)-C(27)	1.569(3)
C(19)-O(4)	1.431(2)
C(19)-C(21)	1.525(3)
C(19)-H(19)	1.0000
C(20)-O(4)	1.407(3)
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-C(22)	1.518(3)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-O(5)	1.445(2)
C(23)-C(31)	1.555(3)
C(23)-C(24)	1.564(3)
C(24)-O(6)	1.426(2)
C(24)-C(25)	1.527(3)
C(24)-C(27)	1.540(3)
C(25)-O(7)	1.426(3)
C(25)-C(29)	1.519(3)
C(25)-H(25)	1.0000
C(26)-O(7)	1.421(2)
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-C(28)	1.570(2)
C(27)-H(27)	1.0000
C(28)-C(29)	1.541(3)
C(28)-H(28A)	0.9900
C(28)-H(28B)	0.9900
C(29)-C(30)	1.530(3)
C(29)-H(29)	1.0000
C(30)-O(8)	1.434(2)
C(30)-C(31)	1.547(3)
C(30)-H(30)	1.0000

C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(32)-O(8)	1.419(3)
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
N(1)-H(1)	0.88(3)
O(5)-H(5A)	0.83(3)
O(6)-H(6A)	0.81(4)
O(9)-H(9)	0.86(3)
O(9)-H(9)#1	0.86(3)

Table 83. Bond angles [°] for s17phar13.

C(2)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
O(1)-C(2)-N(1)	124.1(2)
O(1)-C(2)-C(1)	121.5(2)
N(1)-C(2)-C(1)	114.40(19)
N(1)-C(3)-C(4)	121.97(19)
N(1)-C(3)-C(8)	119.54(18)
C(4)-C(3)-C(8)	118.5(2)
C(5)-C(4)-C(3)	120.6(2)
C(5)-C(4)-H(4)	119.7
C(3)-C(4)-H(4)	119.7
C(4)-C(5)-C(6)	121.4(2)
C(4)-C(5)-H(5)	119.3
C(6)-C(5)-H(5)	119.3
C(5)-C(6)-C(7)	118.8(2)
C(5)-C(6)-H(6)	120.6
C(7)-C(6)-H(6)	120.6
C(6)-C(7)-C(8)	121.4(2)

C(6)-C(7)-H(7)	119.3
C(8)-C(7)-H(7)	119.3
C(7)-C(8)-C(3)	119.15(19)
C(7)-C(8)-C(9)	119.35(19)
C(3)-C(8)-C(9)	121.49(19)
O(2)-C(9)-O(3)	124.15(19)
O(2)-C(9)-C(8)	124.52(19)
O(3)-C(9)-C(8)	111.32(18)
O(3)-C(10)-C(22)	108.98(16)
O(3)-C(10)-C(17)	102.47(15)
C(22)-C(10)-C(17)	110.73(17)
O(3)-C(10)-C(11)	109.62(16)
C(22)-C(10)-C(11)	114.21(17)
C(17)-C(10)-C(11)	110.17(16)
N(2)-C(11)-C(10)	113.31(16)
N(2)-C(11)-H(11A)	108.9
C(10)-C(11)-H(11A)	108.9
N(2)-C(11)-H(11B)	108.9
C(10)-C(11)-H(11B)	108.9
H(11A)-C(11)-H(11B)	107.7
N(2)-C(12)-C(13)	112.87(18)
N(2)-C(12)-H(12A)	109.0
C(13)-C(12)-H(12A)	109.0
N(2)-C(12)-H(12B)	109.0
C(13)-C(12)-H(12B)	109.0
H(12A)-C(12)-H(12B)	107.8
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
N(2)-C(14)-C(18)	110.99(15)
N(2)-C(14)-C(15)	114.87(15)
C(18)-C(14)-C(15)	100.98(15)
N(2)-C(14)-H(14)	109.9
C(18)-C(14)-H(14)	109.9
C(15)-C(14)-H(14)	109.9
C(23)-C(15)-C(16)	111.53(16)

C(23)-C(15)-C(14)	110.87(15)
C(16)-C(15)-C(14)	102.85(15)
C(23)-C(15)-H(15)	110.5
C(16)-C(15)-H(15)	110.5
C(14)-C(15)-H(15)	110.5
C(15)-C(16)-C(17)	104.72(15)
C(15)-C(16)-H(16A)	110.8
C(17)-C(16)-H(16A)	110.8
C(15)-C(16)-H(16B)	110.8
C(17)-C(16)-H(16B)	110.8
H(16A)-C(16)-H(16B)	108.9
C(10)-C(17)-C(16)	108.63(16)
C(10)-C(17)-C(18)	107.83(15)
C(16)-C(17)-C(18)	105.27(15)
C(10)-C(17)-H(17)	111.6
C(16)-C(17)-H(17)	111.6
C(18)-C(17)-H(17)	111.6
C(14)-C(18)-C(19)	118.22(16)
C(14)-C(18)-C(17)	97.85(14)
C(19)-C(18)-C(17)	111.46(15)
C(14)-C(18)-C(27)	109.83(15)
C(19)-C(18)-C(27)	107.50(15)
C(17)-C(18)-C(27)	111.83(15)
O(4)-C(19)-C(21)	107.84(17)
O(4)-C(19)-C(18)	109.57(16)
C(21)-C(19)-C(18)	117.05(16)
O(4)-C(19)-H(19)	107.3
C(21)-C(19)-H(19)	107.3
C(18)-C(19)-H(19)	107.3
O(4)-C(20)-H(20A)	109.5
O(4)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
O(4)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(22)-C(21)-C(19)	111.98(17)
C(22)-C(21)-H(21A)	109.2
C(19)-C(21)-H(21A)	109.2
C(22)-C(21)-H(21B)	109.2

C(19)-C(21)-H(21B)	109.2
H(21A)-C(21)-H(21B)	107.9
C(10)-C(22)-C(21)	108.65(16)
C(10)-C(22)-H(22A)	110.0
C(21)-C(22)-H(22A)	110.0
C(10)-C(22)-H(22B)	110.0
C(21)-C(22)-H(22B)	110.0
H(22A)-C(22)-H(22B)	108.3
O(5)-C(23)-C(15)	106.59(15)
O(5)-C(23)-C(31)	107.28(16)
C(15)-C(23)-C(31)	110.69(16)
O(5)-C(23)-C(24)	108.05(16)
C(15)-C(23)-C(24)	110.34(16)
C(31)-C(23)-C(24)	113.56(15)
O(6)-C(24)-C(25)	110.98(16)
O(6)-C(24)-C(27)	108.66(16)
C(25)-C(24)-C(27)	103.95(16)
O(6)-C(24)-C(23)	112.16(16)
C(25)-C(24)-C(23)	108.80(16)
C(27)-C(24)-C(23)	111.99(17)
O(7)-C(25)-C(29)	117.32(17)
O(7)-C(25)-C(24)	108.81(17)
C(29)-C(25)-C(24)	102.10(16)
O(7)-C(25)-H(25)	109.4
C(29)-C(25)-H(25)	109.4
C(24)-C(25)-H(25)	109.4
O(7)-C(26)-H(26A)	109.5
O(7)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
O(7)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(24)-C(27)-C(18)	117.36(16)
C(24)-C(27)-C(28)	102.94(15)
C(18)-C(27)-C(28)	115.45(16)
C(24)-C(27)-H(27)	106.8
C(18)-C(27)-H(27)	106.8
C(28)-C(27)-H(27)	106.8
C(29)-C(28)-C(27)	107.09(16)

C(29)-C(28)-H(28A)	110.3
C(27)-C(28)-H(28A)	110.3
C(29)-C(28)-H(28B)	110.3
C(27)-C(28)-H(28B)	110.3
H(28A)-C(28)-H(28B)	108.6
C(25)-C(29)-C(30)	112.27(17)
C(25)-C(29)-C(28)	100.71(16)
C(30)-C(29)-C(28)	110.65(17)
C(25)-C(29)-H(29)	110.9
C(30)-C(29)-H(29)	110.9
C(28)-C(29)-H(29)	110.9
O(8)-C(30)-C(29)	107.37(16)
O(8)-C(30)-C(31)	109.60(16)
C(29)-C(30)-C(31)	113.41(16)
O(8)-C(30)-H(30)	108.8
C(29)-C(30)-H(30)	108.8
C(31)-C(30)-H(30)	108.8
C(30)-C(31)-C(23)	118.67(16)
C(30)-C(31)-H(31A)	107.6
C(23)-C(31)-H(31A)	107.6
C(30)-C(31)-H(31B)	107.6
C(23)-C(31)-H(31B)	107.6
H(31A)-C(31)-H(31B)	107.1
O(8)-C(32)-H(32A)	109.5
O(8)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
O(8)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(2)-N(1)-C(3)	128.50(18)
C(2)-N(1)-H(1)	116.8(19)
C(3)-N(1)-H(1)	114.5(19)
C(12)-N(2)-C(14)	111.70(16)
C(12)-N(2)-C(11)	110.13(15)
C(14)-N(2)-C(11)	116.44(15)
C(9)-O(3)-C(10)	121.06(16)
C(20)-O(4)-C(19)	113.8(2)
C(23)-O(5)-H(5A)	102(2)
C(24)-O(6)-H(6A)	108(2)
C(26)-O(7)-C(25)	112.98(17)
C(32)-O(8)-C(30)	111.76(17)

H(9)-O(9)-H(9)#1 115(9)

Symmetry transformations used to generate equivalent atoms: #1 x-y,-y,-z+2/3

Table 84. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for s17phar13. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	40(1)	29(1)	30(1)	6(1)	5(1)	17(1)
C(2)	34(1)	31(1)	21(1)	5(1)	4(1)	22(1)
C(3)	20(1)	27(1)	17(1)	2(1)	1(1)	15(1)
C(4)	29(1)	33(1)	18(1)	0(1)	1(1)	19(1)
C(5)	34(1)	34(1)	21(1)	-8(1)	-4(1)	21(1)
C(6)	30(1)	24(1)	28(1)	-6(1)	-3(1)	13(1)
C(7)	25(1)	25(1)	22(1)	0(1)	1(1)	13(1)
C(8)	20(1)	23(1)	18(1)	1(1)	0(1)	12(1)
C(9)	23(1)	22(1)	17(1)	4(1)	1(1)	12(1)
C(10)	21(1)	18(1)	13(1)	1(1)	-1(1)	7(1)
C(11)	20(1)	19(1)	16(1)	2(1)	2(1)	7(1)
C(12)	16(1)	21(1)	21(1)	0(1)	-1(1)	7(1)
C(13)	20(1)	26(1)	34(1)	2(1)	-2(1)	5(1)
C(14)	16(1)	13(1)	14(1)	0(1)	1(1)	6(1)
C(15)	18(1)	16(1)	16(1)	1(1)	3(1)	7(1)
C(16)	23(1)	16(1)	15(1)	1(1)	3(1)	8(1)
C(17)	18(1)	16(1)	15(1)	0(1)	-1(1)	6(1)
C(18)	18(1)	16(1)	14(1)	1(1)	0(1)	7(1)
C(19)	20(1)	19(1)	18(1)	-1(1)	0(1)	11(1)
C(20)	82(2)	50(2)	36(1)	-10(1)	8(1)	44(2)
C(21)	24(1)	15(1)	24(1)	1(1)	0(1)	9(1)
C(22)	24(1)	21(1)	21(1)	4(1)	-1(1)	12(1)
C(23)	22(1)	15(1)	16(1)	0(1)	3(1)	9(1)
C(24)	17(1)	18(1)	15(1)	1(1)	0(1)	6(1)
C(25)	17(1)	21(1)	20(1)	4(1)	3(1)	8(1)
C(26)	33(1)	27(1)	33(1)	15(1)	10(1)	12(1)
C(27)	14(1)	18(1)	17(1)	2(1)	1(1)	7(1)
C(28)	21(1)	22(1)	17(1)	2(1)	4(1)	12(1)
C(29)	19(1)	22(1)	17(1)	3(1)	5(1)	10(1)

C(30)	18(1)	21(1)	17(1)	0(1)	1(1)	9(1)
C(31)	18(1)	22(1)	18(1)	4(1)	2(1)	11(1)
C(32)	32(1)	53(2)	26(1)	3(1)	-6(1)	24(1)
N(1)	25(1)	26(1)	16(1)	2(1)	1(1)	12(1)
N(2)	15(1)	17(1)	16(1)	1(1)	0(1)	6(1)
O(1)	69(1)	36(1)	20(1)	5(1)	3(1)	25(1)
O(2)	28(1)	21(1)	18(1)	1(1)	1(1)	6(1)
O(3)	25(1)	19(1)	15(1)	1(1)	-1(1)	7(1)
O(4)	45(1)	24(1)	18(1)	-3(1)	0(1)	19(1)
O(5)	30(1)	15(1)	24(1)	1(1)	8(1)	10(1)
O(6)	25(1)	20(1)	20(1)	-2(1)	-5(1)	6(1)
O(7)	24(1)	18(1)	22(1)	6(1)	4(1)	7(1)
O(8)	26(1)	40(1)	17(1)	7(1)	1(1)	19(1)
O(9)	52(3)	87(6)	95(6)	-67(5)	-34(2)	44(3)

Table 85. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{3}) for s17phar13.

	x	y	z	U(eq)
H(1A)	8597	12149	2009	49
H(1B)	9863	11778	2032	49
H(1C)	8845	11522	2319	49
H(4)	6463	7297	1732	30
H(5)	4814	4869	1702	34
H(6)	3637	3545	2135	34
H(7)	4200	4679	2609	29
H(11A)	7223	6847	3306	23
H(11B)	7446	8412	3369	23
H(12A)	8435	6610	3707	25
H(12B)	8306	7094	4044	25
H(13A)	10433	8915	3855	44
H(13B)	9353	9535	3850	44
H(13C)	9692	8965	3542	44
H(14)	5847	5855	4106	18
H(15)	6415	4463	3710	20

H(16A)	3970	3399	3387	23
H(16B)	5488	4672	3263	23
H(17)	3230	5056	3378	21
H(19)	3072	6797	3858	22
H(20A)	4084	8474	4522	77
H(20B)	2911	7893	4256	77
H(20C)	4418	9338	4208	77
H(21A)	4561	9070	3695	25
H(21B)	5967	8923	3729	25
H(22A)	3815	7566	3267	26
H(22B)	5439	8828	3211	26
H(25)	1188	1954	4247	24
H(26A)	1590	-831	4521	48
H(26B)	535	-181	4516	48
H(26C)	1982	585	4713	48
H(27)	2108	4336	3908	21
H(28A)	3883	5560	4406	24
H(28B)	2154	4691	4403	24
H(29)	2483	3093	4686	23
H(30)	5196	4703	4580	23
H(31A)	5100	2320	4300	23
H(31B)	6204	3979	4241	23
H(32A)	5916	2749	5082	54
H(32B)	6493	4300	4933	54
H(32C)	6461	3028	4737	54
H(1)	7460(30)	9310(30)	2405(6)	28(7)
H(5A)	3800(30)	1230(30)	3913(7)	31(8)
H(6A)	2190(40)	1580(40)	3661(8)	48(10)
H(9)	3460(50)	630(60)	3431(14)	48(18)

Table 86. Torsion angles [°] for s17phar13.

N(1)-C(3)-C(4)-C(5)	-178.5(2)
C(8)-C(3)-C(4)-C(5)	2.6(3)
C(3)-C(4)-C(5)-C(6)	-0.6(3)
C(4)-C(5)-C(6)-C(7)	-1.4(4)

C(5)-C(6)-C(7)-C(8)	1.3(3)
C(6)-C(7)-C(8)-C(3)	0.8(3)
C(6)-C(7)-C(8)-C(9)	-178.6(2)
N(1)-C(3)-C(8)-C(7)	178.41(19)
C(4)-C(3)-C(8)-C(7)	-2.7(3)
N(1)-C(3)-C(8)-C(9)	-2.2(3)
C(4)-C(3)-C(8)-C(9)	176.71(19)
C(7)-C(8)-C(9)-O(2)	174.3(2)
C(3)-C(8)-C(9)-O(2)	-5.1(3)
C(7)-C(8)-C(9)-O(3)	-5.1(3)
C(3)-C(8)-C(9)-O(3)	175.43(18)
O(3)-C(10)-C(11)-N(2)	-152.18(16)
C(22)-C(10)-C(11)-N(2)	85.2(2)
C(17)-C(10)-C(11)-N(2)	-40.2(2)
N(2)-C(14)-C(15)-C(23)	165.97(16)
C(18)-C(14)-C(15)-C(23)	-74.55(18)
N(2)-C(14)-C(15)-C(16)	-74.70(19)
C(18)-C(14)-C(15)-C(16)	44.78(17)
C(23)-C(15)-C(16)-C(17)	100.82(17)
C(14)-C(15)-C(16)-C(17)	-18.05(19)
O(3)-C(10)-C(17)-C(16)	65.40(18)
C(22)-C(10)-C(17)-C(16)	-178.50(16)
C(11)-C(10)-C(17)-C(16)	-51.2(2)
O(3)-C(10)-C(17)-C(18)	178.99(15)
C(22)-C(10)-C(17)-C(18)	-64.9(2)
C(11)-C(10)-C(17)-C(18)	62.4(2)
C(15)-C(16)-C(17)-C(10)	100.94(17)
C(15)-C(16)-C(17)-C(18)	-14.33(19)
N(2)-C(14)-C(18)-C(19)	-49.5(2)
C(15)-C(14)-C(18)-C(19)	-171.73(15)
N(2)-C(14)-C(18)-C(17)	70.05(17)
C(15)-C(14)-C(18)-C(17)	-52.18(16)
N(2)-C(14)-C(18)-C(27)	-173.29(14)
C(15)-C(14)-C(18)-C(27)	64.48(17)
C(10)-C(17)-C(18)-C(14)	-74.55(18)
C(16)-C(17)-C(18)-C(14)	41.27(17)
C(10)-C(17)-C(18)-C(19)	50.0(2)
C(16)-C(17)-C(18)-C(19)	165.82(16)
C(10)-C(17)-C(18)-C(27)	170.36(16)

C(16)-C(17)-C(18)-C(27)	-73.82(19)
C(14)-C(18)-C(19)-O(4)	-52.8(2)
C(17)-C(18)-C(19)-O(4)	-165.02(16)
C(27)-C(18)-C(19)-O(4)	72.1(2)
C(14)-C(18)-C(19)-C(21)	70.3(2)
C(17)-C(18)-C(19)-C(21)	-41.9(2)
C(27)-C(18)-C(19)-C(21)	-164.77(17)
O(4)-C(19)-C(21)-C(22)	167.85(17)
C(18)-C(19)-C(21)-C(22)	43.8(2)
O(3)-C(10)-C(22)-C(21)	179.42(16)
C(17)-C(10)-C(22)-C(21)	67.4(2)
C(11)-C(10)-C(22)-C(21)	-57.6(2)
C(19)-C(21)-C(22)-C(10)	-54.4(2)
C(16)-C(15)-C(23)-O(5)	66.6(2)
C(14)-C(15)-C(23)-O(5)	-179.44(15)
C(16)-C(15)-C(23)-C(31)	-177.07(16)
C(14)-C(15)-C(23)-C(31)	-63.1(2)
C(16)-C(15)-C(23)-C(24)	-50.5(2)
C(14)-C(15)-C(23)-C(24)	63.5(2)
O(5)-C(23)-C(24)-O(6)	-34.6(2)
C(15)-C(23)-C(24)-O(6)	81.6(2)
C(31)-C(23)-C(24)-O(6)	-153.49(16)
O(5)-C(23)-C(24)-C(25)	88.55(19)
C(15)-C(23)-C(24)-C(25)	-155.27(16)
C(31)-C(23)-C(24)-C(25)	-30.3(2)
O(5)-C(23)-C(24)-C(27)	-157.10(15)
C(15)-C(23)-C(24)-C(27)	-40.9(2)
C(31)-C(23)-C(24)-C(27)	84.0(2)
O(6)-C(24)-C(25)-O(7)	72.9(2)
C(27)-C(24)-C(25)-O(7)	-170.49(16)
C(23)-C(24)-C(25)-O(7)	-51.0(2)
O(6)-C(24)-C(25)-C(29)	-162.46(17)
C(27)-C(24)-C(25)-C(29)	-45.81(19)
C(23)-C(24)-C(25)-C(29)	73.67(19)
O(6)-C(24)-C(27)-C(18)	-88.3(2)
C(25)-C(24)-C(27)-C(18)	153.50(16)
C(23)-C(24)-C(27)-C(18)	36.2(2)
O(6)-C(24)-C(27)-C(28)	143.77(16)
C(25)-C(24)-C(27)-C(28)	25.52(19)

C(23)-C(24)-C(27)-C(28)	-91.77(18)
C(14)-C(18)-C(27)-C(24)	-50.7(2)
C(19)-C(18)-C(27)-C(24)	179.43(16)
C(17)-C(18)-C(27)-C(24)	56.8(2)
C(14)-C(18)-C(27)-C(28)	71.0(2)
C(19)-C(18)-C(27)-C(28)	-58.9(2)
C(17)-C(18)-C(27)-C(28)	178.48(16)
C(24)-C(27)-C(28)-C(29)	3.2(2)
C(18)-C(27)-C(28)-C(29)	-125.99(18)
O(7)-C(25)-C(29)-C(30)	47.4(2)
C(24)-C(25)-C(29)-C(30)	-71.4(2)
O(7)-C(25)-C(29)-C(28)	165.16(16)
C(24)-C(25)-C(29)-C(28)	46.35(19)
C(27)-C(28)-C(29)-C(25)	-30.50(19)
C(27)-C(28)-C(29)-C(30)	88.42(19)
C(25)-C(29)-C(30)-O(8)	-97.42(19)
C(28)-C(29)-C(30)-O(8)	150.93(16)
C(25)-C(29)-C(30)-C(31)	23.8(2)
C(28)-C(29)-C(30)-C(31)	-87.8(2)
O(8)-C(30)-C(31)-C(23)	141.52(18)
C(29)-C(30)-C(31)-C(23)	21.6(3)
O(5)-C(23)-C(31)-C(30)	-137.16(18)
C(15)-C(23)-C(31)-C(30)	106.9(2)
C(24)-C(23)-C(31)-C(30)	-17.8(3)
O(1)-C(2)-N(1)-C(3)	0.3(4)
C(1)-C(2)-N(1)-C(3)	-179.7(2)
C(4)-C(3)-N(1)-C(2)	11.6(3)
C(8)-C(3)-N(1)-C(2)	-169.5(2)
C(13)-C(12)-N(2)-C(14)	-165.45(17)
C(13)-C(12)-N(2)-C(11)	63.5(2)
C(18)-C(14)-N(2)-C(12)	177.17(15)
C(15)-C(14)-N(2)-C(12)	-69.1(2)
C(18)-C(14)-N(2)-C(11)	-55.1(2)
C(15)-C(14)-N(2)-C(11)	58.6(2)
C(10)-C(11)-N(2)-C(12)	165.29(17)
C(10)-C(11)-N(2)-C(14)	36.8(2)
O(2)-C(9)-O(3)-C(10)	1.7(3)
C(8)-C(9)-O(3)-C(10)	-178.84(17)
C(22)-C(10)-O(3)-C(9)	65.7(2)

C(17)-C(10)-O(3)-C(9)	-176.97(17)
C(11)-C(10)-O(3)-C(9)	-60.0(2)
C(21)-C(19)-O(4)-C(20)	74.6(3)
C(18)-C(19)-O(4)-C(20)	-157.0(2)
C(29)-C(25)-O(7)-C(26)	69.5(2)
C(24)-C(25)-O(7)-C(26)	-175.37(18)
C(29)-C(30)-O(8)-C(32)	-168.23(18)
C(31)-C(30)-O(8)-C(32)	68.2(2)

Symmetry transformations used to generate equivalent atoms:

#1 x-y,-y,-z+2/3

Table 87. Hydrogen bonds for s17phar13 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1)...O(2)	0.88(3)	1.94(3)	2.670(2)	139(3)
O(5)-H(5A)...O(7)	0.83(3)	2.16(3)	2.831(2)	138(3)
O(6)-H(6A)...O(5)	0.81(4)	2.24(4)	2.673(2)	114(3)
O(6)-H(6A)...O(9)	0.81(4)	2.49(4)	3.249(4)	155(3)
O(9)-H(9)...O(5)	0.86(3)	1.99(4)	2.768(2)	151(6)

Symmetry transformations used to generate equivalent atoms:

#1 x-y,-y,-z+2/3

e17phar1: crassicauline A (**28**)

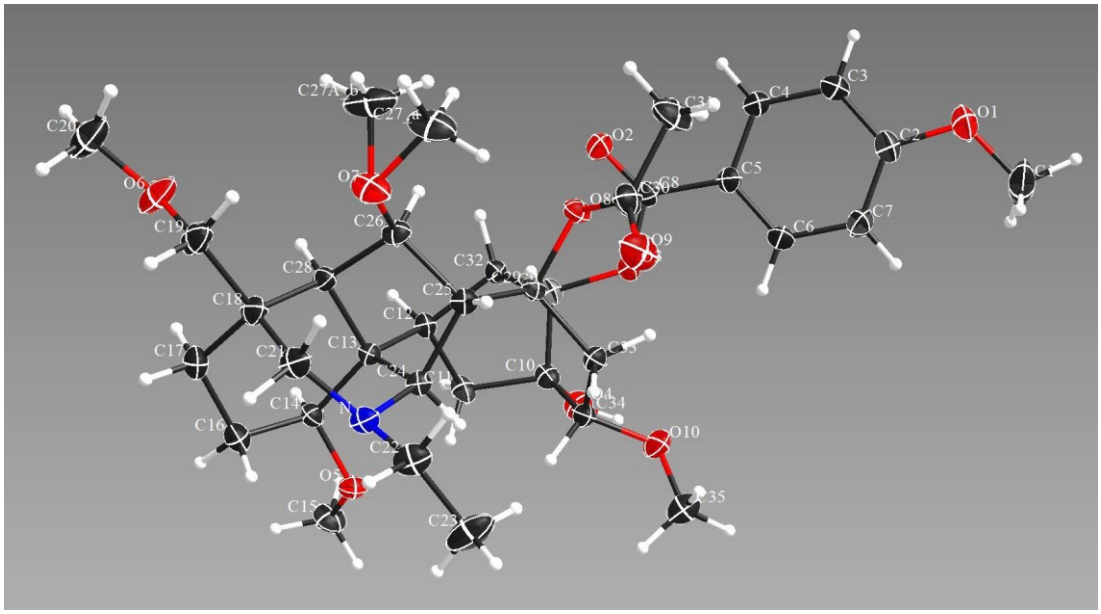

Table 88. Crystal data and structure refinement for e17phar1.

Identification code	e17phar1	
Empirical formula	C35 H49 N O10	
Formula weight	643.75	
Temperature	150.01(10) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 9.39880(10) Å	α= 90°.
	b = 15.4136(2) Å	β= 92.1560(10)°.
	c = 11.4006(2) Å	γ = 90°.
Volume	1650.43(4) $Å^3$	
Z	2	
Density (calculated)	1.295 Mg/m^3	
Absorption coefficient	0.094 mm^{-1}	
F(000)	692	
Crystal size	0.600 x 0.500 x 0.180 mm^3	
Theta range for data collection	3.420 to 30.752°.	
Index ranges	-13<=h<=13, -21<=k<=21, -16<=l<=16	
Reflections collected	97148	
Independent reflections	9254 [R(int) = 0.0371]	

Completeness to theta = 1.000°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.90805
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9254 / 1 / 437
Goodness-of-fit on F^2	1.023
Final R indices [I>2sigma(I)]	R1 = 0.0388, wR2 = 0.0912
R indices (all data)	R1 = 0.0444, wR2 = 0.0940
Absolute structure parameter	-0.20(15)
Extinction coefficient	n/a
Largest diff. peak and hole	0.293 and -0.231 e.$Å^{-3}$

Table 89. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for e17phar1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N	2931(2)	4651(1)	7227(1)	20(1)
O(1)	10076(2)	3203(1)	-776(2)	36(1)
O(2)	7560(2)	6195(1)	2376(1)	29(1)
O(3)	5692(1)	5290(1)	2154(1)	20(1)
O(4)	2638(2)	5658(1)	1646(1)	28(1)
O(5)	739(1)	5878(1)	5534(1)	21(1)
O(6)	5221(2)	7200(1)	9101(1)	36(1)
O(7)	6610(1)	5307(1)	7592(1)	30(1)
O(8)	6901(1)	4740(1)	4432(1)	19(1)
O(9)	6948(2)	3338(1)	5005(2)	35(1)
O(10)	3001(2)	4041(1)	2083(1)	30(1)
C(1)	9412(4)	2468(2)	-1325(3)	58(1)
C(2)	9254(2)	3729(1)	-125(2)	24(1)
C(3)	9931(2)	4462(2)	330(2)	30(1)
C(4)	9211(2)	5041(1)	1009(2)	27(1)
C(5)	7778(2)	4901(1)	1240(2)	19(1)
C(6)	7108(2)	4168(1)	781(2)	24(1)
C(7)	7833(2)	3581(1)	99(2)	28(1)
C(8)	7042(2)	5538(1)	1978(2)	20(1)
C(9)	4827(2)	5838(1)	2863(2)	18(1)

C(10)	3304(2)	5518(1)	2770(2)	21(1)
C(11)	2621(2)	6087(1)	3683(2)	23(1)
C(12)	3768(2)	6219(1)	4702(1)	15(1)
C(13)	3331(2)	5928(1)	5964(1)	15(1)
C(14)	1849(2)	6327(1)	6202(2)	19(1)
C(15)	-348(2)	6445(2)	5099(2)	30(1)
C(16)	1399(2)	6313(2)	7472(2)	27(1)
C(17)	2613(2)	6572(2)	8304(2)	30(1)
C(18)	3949(2)	6021(1)	8150(2)	22(1)
C(19)	4982(2)	6286(1)	9166(2)	28(1)
C(20)	5923(3)	7522(2)	10125(2)	43(1)
C(21)	3652(2)	5041(1)	8271(2)	24(1)
C(22)	2903(2)	3706(1)	7359(2)	25(1)
C(23)	1920(3)	3250(2)	6478(2)	38(1)
C(24)	3445(2)	4940(1)	6091(2)	15(1)
C(25)	5059(2)	4806(1)	5917(2)	16(1)
C(26)	5772(2)	5579(1)	6591(2)	19(1)
C(27)	7924(3)	4941(2)	7322(3)	34(1)
C(27A)	7922(12)	5565(10)	7752(11)	40(4)
C(28)	4517(2)	6189(1)	6909(2)	17(1)
C(29)	5358(2)	4856(1)	4609(2)	16(1)
C(30)	7533(2)	3968(1)	4627(2)	25(1)
C(31)	9062(2)	4009(2)	4288(2)	35(1)
C(32)	5132(2)	5796(1)	4192(1)	15(1)
C(33)	4517(2)	4191(1)	3838(2)	19(1)
C(34)	3203(2)	4543(1)	3131(2)	21(1)
C(35)	2296(3)	3240(2)	2275(2)	37(1)

Table 90. Bond lengths [Å] for e17phar1.

N-C(22)	1.465(2)
N-C(24)	1.468(2)
N-C(21)	1.476(2)
O(1)-C(2)	1.359(2)
O(1)-C(1)	1.427(3)
O(2)-C(8)	1.206(2)

O(3)-C(8)	1.347(2)
O(3)-C(9)	1.441(2)
O(4)-C(10)	1.422(2)
O(4)-H(4A)	0.80(3)
O(5)-C(15)	1.419(2)
O(5)-C(14)	1.444(2)
O(6)-C(20)	1.410(3)
O(6)-C(19)	1.428(3)
O(7)-C(27A)	1.302(11)
O(7)-C(27)	1.402(3)
O(7)-C(26)	1.425(2)
O(8)-C(30)	1.345(2)
O(8)-C(29)	1.482(2)
O(9)-C(30)	1.203(3)
O(10)-C(35)	1.422(3)
O(10)-C(34)	1.431(2)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(2)-C(7)	1.387(3)
C(2)-C(3)	1.388(3)
C(3)-C(4)	1.377(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.399(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.387(3)
C(5)-C(8)	1.481(2)
C(6)-C(7)	1.389(3)
C(6)-H(6)	0.9500
C(7)-H(7)	0.9500
C(9)-C(10)	1.514(2)
C(9)-C(32)	1.533(2)
C(9)-H(9)	1.0000
C(10)-C(11)	1.521(3)
C(10)-C(34)	1.561(3)
C(11)-C(12)	1.568(2)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(32)	1.569(2)

C(12)-C(13)	1.576(2)
C(12)-H(12)	1.0000
C(13)-C(24)	1.532(2)
C(13)-C(14)	1.556(2)
C(13)-C(28)	1.573(2)
C(14)-C(16)	1.524(3)
C(14)-H(14)	1.0000
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-C(17)	1.509(3)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.532(3)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-C(19)	1.538(3)
C(18)-C(21)	1.542(3)
C(18)-C(28)	1.553(2)
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-C(23)	1.512(3)
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-C(25)	1.552(2)
C(24)-H(24)	1.0000
C(25)-C(29)	1.530(2)
C(25)-C(26)	1.557(2)
C(25)-H(25)	1.0000
C(26)-C(28)	1.561(3)
C(26)-H(26)	1.0000

C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(27A)-H(27D)	0.9800
C(27A)-H(27E)	0.9800
C(27A)-H(27F)	0.9800
C(28)-H(28)	1.0000
C(29)-C(32)	1.537(2)
C(29)-C(33)	1.548(2)
C(30)-C(31)	1.504(3)
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32)	1.0000
C(33)-C(34)	1.546(3)
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(34)-H(34)	1.0000
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800

Table 91. Bond angles [°] for e17phar1.

C(22)-N-C(24)	113.62(15)
C(22)-N-C(21)	109.39(14)
C(24)-N-C(21)	115.53(14)
C(2)-O(1)-C(1)	117.64(19)
C(8)-O(3)-C(9)	118.18(14)
C(10)-O(4)-H(4A)	102(2)
C(15)-O(5)-C(14)	112.72(15)
C(20)-O(6)-C(19)	111.94(18)
C(27A)-O(7)-C(26)	120.9(5)
C(27)-O(7)-C(26)	114.06(17)
C(30)-O(8)-C(29)	120.78(14)
C(35)-O(10)-C(34)	112.89(16)

O(1)-C(1)-H(1A)	109.5
O(1)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
O(1)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
O(1)-C(2)-C(7)	125.01(19)
O(1)-C(2)-C(3)	115.27(18)
C(7)-C(2)-C(3)	119.73(18)
C(4)-C(3)-C(2)	120.69(18)
C(4)-C(3)-H(3)	119.7
C(2)-C(3)-H(3)	119.7
C(3)-C(4)-C(5)	120.16(18)
C(3)-C(4)-H(4)	119.9
C(5)-C(4)-H(4)	119.9
C(6)-C(5)-C(4)	118.82(17)
C(6)-C(5)-C(8)	122.61(16)
C(4)-C(5)-C(8)	118.57(16)
C(5)-C(6)-C(7)	121.12(17)
C(5)-C(6)-H(6)	119.4
C(7)-C(6)-H(6)	119.4
C(2)-C(7)-C(6)	119.47(18)
C(2)-C(7)-H(7)	120.3
C(6)-C(7)-H(7)	120.3
O(2)-C(8)-O(3)	123.43(17)
O(2)-C(8)-C(5)	125.45(17)
O(3)-C(8)-C(5)	111.12(15)
O(3)-C(9)-C(10)	108.75(14)
O(3)-C(9)-C(32)	116.16(14)
C(10)-C(9)-C(32)	101.31(13)
O(3)-C(9)-H(9)	110.1
C(10)-C(9)-H(9)	110.1
C(32)-C(9)-H(9)	110.1
O(4)-C(10)-C(9)	113.33(15)
O(4)-C(10)-C(11)	110.21(15)
C(9)-C(10)-C(11)	100.74(15)
O(4)-C(10)-C(34)	110.82(16)
C(9)-C(10)-C(34)	111.22(15)
C(11)-C(10)-C(34)	110.09(15)

C(10)-C(11)-C(12)	106.59(14)
C(10)-C(11)-H(11A)	110.4
C(12)-C(11)-H(11A)	110.4
C(10)-C(11)-H(11B)	110.4
C(12)-C(11)-H(11B)	110.4
H(11A)-C(11)-H(11B)	108.6
C(11)-C(12)-C(32)	102.69(13)
C(11)-C(12)-C(13)	116.38(14)
C(32)-C(12)-C(13)	117.70(13)
C(11)-C(12)-H(12)	106.4
C(32)-C(12)-H(12)	106.4
C(13)-C(12)-H(12)	106.4
C(24)-C(13)-C(14)	115.84(14)
C(24)-C(13)-C(28)	98.32(13)
C(14)-C(13)-C(28)	113.32(14)
C(24)-C(13)-C(12)	110.43(13)
C(14)-C(13)-C(12)	108.19(13)
C(28)-C(13)-C(12)	110.48(13)
O(5)-C(14)-C(16)	105.90(14)
O(5)-C(14)-C(13)	110.66(14)
C(16)-C(14)-C(13)	116.25(15)
O(5)-C(14)-H(14)	107.9
C(16)-C(14)-H(14)	107.9
C(13)-C(14)-H(14)	107.9
O(5)-C(15)-H(15A)	109.5
O(5)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
O(5)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(17)-C(16)-C(14)	111.29(16)
C(17)-C(16)-H(16A)	109.4
C(14)-C(16)-H(16A)	109.4
C(17)-C(16)-H(16B)	109.4
C(14)-C(16)-H(16B)	109.4
H(16A)-C(16)-H(16B)	108.0
C(16)-C(17)-C(18)	112.67(17)
C(16)-C(17)-H(17A)	109.1
C(18)-C(17)-H(17A)	109.1

C(16)-C(17)-H(17B)	109.1
C(18)-C(17)-H(17B)	109.1
H(17A)-C(17)-H(17B)	107.8
C(17)-C(18)-C(19)	105.25(16)
C(17)-C(18)-C(21)	112.38(16)
C(19)-C(18)-C(21)	107.71(16)
C(17)-C(18)-C(28)	108.84(16)
C(19)-C(18)-C(28)	114.38(15)
C(21)-C(18)-C(28)	108.35(15)
O(6)-C(19)-C(18)	108.60(17)
O(6)-C(19)-H(19A)	110.0
C(18)-C(19)-H(19A)	110.0
O(6)-C(19)-H(19B)	110.0
C(18)-C(19)-H(19B)	110.0
H(19A)-C(19)-H(19B)	108.4
O(6)-C(20)-H(20A)	109.5
O(6)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
O(6)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
N-C(21)-C(18)	113.96(15)
N-C(21)-H(21A)	108.8
C(18)-C(21)-H(21A)	108.8
N-C(21)-H(21B)	108.8
C(18)-C(21)-H(21B)	108.8
H(21A)-C(21)-H(21B)	107.7
N-C(22)-C(23)	113.98(16)
N-C(22)-H(22A)	108.8
C(23)-C(22)-H(22A)	108.8
N-C(22)-H(22B)	108.8
C(23)-C(22)-H(22B)	108.8
H(22A)-C(22)-H(22B)	107.7
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5

N-C(24)-C(13)	111.16(14)
N-C(24)-C(25)	115.34(14)
C(13)-C(24)-C(25)	100.72(13)
N-C(24)-H(24)	109.8
C(13)-C(24)-H(24)	109.8
C(25)-C(24)-H(24)	109.8
C(29)-C(25)-C(24)	109.55(13)
C(29)-C(25)-C(26)	110.55(13)
C(24)-C(25)-C(26)	103.83(14)
C(29)-C(25)-H(25)	110.9
C(24)-C(25)-H(25)	110.9
C(26)-C(25)-H(25)	110.9
O(7)-C(26)-C(25)	112.61(15)
O(7)-C(26)-C(28)	113.02(14)
C(25)-C(26)-C(28)	105.13(13)
O(7)-C(26)-H(26)	108.6
C(25)-C(26)-H(26)	108.6
C(28)-C(26)-H(26)	108.6
O(7)-C(27)-H(27A)	109.5
O(7)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
O(7)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
O(7)-C(27A)-H(27D)	109.5
O(7)-C(27A)-H(27E)	109.5
H(27D)-C(27A)-H(27E)	109.5
O(7)-C(27A)-H(27F)	109.5
H(27D)-C(27A)-H(27F)	109.5
H(27E)-C(27A)-H(27F)	109.5
C(18)-C(28)-C(26)	113.54(14)
C(18)-C(28)-C(13)	108.77(13)
C(26)-C(28)-C(13)	102.06(13)
C(18)-C(28)-H(28)	110.7
C(26)-C(28)-H(28)	110.7
C(13)-C(28)-H(28)	110.7
O(8)-C(29)-C(25)	110.09(13)
O(8)-C(29)-C(32)	101.32(13)
C(25)-C(29)-C(32)	108.72(13)

O(8)-C(29)-C(33)	108.92(13)
C(25)-C(29)-C(33)	114.30(14)
C(32)-C(29)-C(33)	112.71(14)
O(9)-C(30)-O(8)	124.69(18)
O(9)-C(30)-C(31)	125.43(18)
O(8)-C(30)-C(31)	109.88(17)
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(9)-C(32)-C(29)	111.38(14)
C(9)-C(32)-C(12)	102.94(13)
C(29)-C(32)-C(12)	112.48(13)
C(9)-C(32)-H(32)	110.0
C(29)-C(32)-H(32)	110.0
C(12)-C(32)-H(32)	110.0
C(34)-C(33)-C(29)	116.39(15)
C(34)-C(33)-H(33A)	108.2
C(29)-C(33)-H(33A)	108.2
C(34)-C(33)-H(33B)	108.2
C(29)-C(33)-H(33B)	108.2
H(33A)-C(33)-H(33B)	107.3
O(10)-C(34)-C(33)	108.90(15)
O(10)-C(34)-C(10)	107.91(15)
C(33)-C(34)-C(10)	114.80(15)
O(10)-C(34)-H(34)	108.4
C(33)-C(34)-H(34)	108.4
C(10)-C(34)-H(34)	108.4
O(10)-C(35)-H(35A)	109.5
O(10)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
O(10)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5

Table 92. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for e17phar1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N	22(1)	22(1)	16(1)	3(1)	0(1)	-5(1)
O(1)	34(1)	34(1)	41(1)	-12(1)	14(1)	2(1)
O(2)	28(1)	25(1)	35(1)	-10(1)	8(1)	-7(1)
O(3)	19(1)	23(1)	19(1)	-4(1)	5(1)	-2(1)
O(4)	27(1)	42(1)	17(1)	0(1)	-5(1)	3(1)
O(5)	16(1)	21(1)	26(1)	2(1)	-1(1)	0(1)
O(6)	49(1)	38(1)	21(1)	-1(1)	-9(1)	-17(1)
O(7)	20(1)	49(1)	19(1)	8(1)	-5(1)	3(1)
O(8)	14(1)	17(1)	26(1)	2(1)	2(1)	2(1)
O(9)	31(1)	17(1)	59(1)	6(1)	8(1)	4(1)
O(10)	30(1)	36(1)	25(1)	-10(1)	0(1)	-8(1)
C(1)	67(2)	32(1)	77(2)	-26(1)	44(2)	-12(1)
C(2)	25(1)	26(1)	22(1)	-1(1)	5(1)	4(1)
C(3)	18(1)	38(1)	35(1)	-10(1)	5(1)	-3(1)
C(4)	20(1)	31(1)	31(1)	-11(1)	4(1)	-6(1)
C(5)	19(1)	22(1)	16(1)	0(1)	1(1)	-2(1)
C(6)	21(1)	25(1)	27(1)	-4(1)	7(1)	-5(1)
C(7)	30(1)	23(1)	31(1)	-7(1)	8(1)	-6(1)
C(8)	20(1)	22(1)	18(1)	1(1)	2(1)	-1(1)
C(9)	19(1)	20(1)	16(1)	1(1)	2(1)	2(1)
C(10)	17(1)	29(1)	15(1)	0(1)	-1(1)	4(1)
C(11)	18(1)	32(1)	17(1)	0(1)	-2(1)	9(1)
C(12)	17(1)	14(1)	15(1)	1(1)	1(1)	3(1)
C(13)	14(1)	16(1)	15(1)	0(1)	1(1)	0(1)
C(14)	15(1)	18(1)	23(1)	-2(1)	3(1)	1(1)
C(15)	19(1)	37(1)	35(1)	2(1)	-2(1)	7(1)
C(16)	22(1)	35(1)	25(1)	-6(1)	6(1)	0(1)
C(17)	29(1)	39(1)	22(1)	-11(1)	4(1)	-1(1)
C(18)	23(1)	29(1)	15(1)	-2(1)	1(1)	-5(1)
C(19)	33(1)	34(1)	16(1)	-2(1)	-1(1)	-9(1)
C(20)	57(2)	45(1)	26(1)	-6(1)	-10(1)	-16(1)
C(21)	27(1)	31(1)	15(1)	4(1)	1(1)	-7(1)
C(22)	29(1)	23(1)	23(1)	9(1)	-3(1)	-5(1)
C(23)	53(2)	26(1)	35(1)	9(1)	-11(1)	-16(1)

C(24)	16(1)	15(1)	15(1)	2(1)	0(1)	0(1)
C(25)	17(1)	15(1)	18(1)	3(1)	-1(1)	1(1)
C(26)	17(1)	22(1)	16(1)	3(1)	-2(1)	-1(1)
C(27)	21(1)	51(2)	31(2)	15(1)	-7(1)	3(1)
C(27A)	28(5)	51(8)	42(7)	11(6)	-9(4)	-17(5)
C(28)	17(1)	19(1)	15(1)	-1(1)	-1(1)	-2(1)
C(29)	12(1)	15(1)	20(1)	2(1)	1(1)	2(1)
C(30)	21(1)	19(1)	34(1)	-1(1)	1(1)	5(1)
C(31)	21(1)	31(1)	52(1)	5(1)	5(1)	9(1)
C(32)	16(1)	14(1)	16(1)	1(1)	2(1)	1(1)
C(33)	18(1)	17(1)	23(1)	-2(1)	2(1)	-1(1)
C(34)	17(1)	27(1)	18(1)	-4(1)	2(1)	-2(1)
C(35)	33(1)	33(1)	45(1)	-11(1)	1(1)	-8(1)

Table 93. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for e17phar1.

	x	y	z	U(eq)
H(4A)	2680(30)	5190(20)	1350(30)	43(8)
H(1A)	10105	2163	-1796	87
H(1B)	8610	2661	-1833	87
H(1C)	9066	2076	-721	87
H(3)	10902	4564	172	36
H(4)	9688	5538	1322	33
H(6)	6137	4065	937	29
H(7)	7361	3082	-213	33
H(9)	4878	6452	2586	22
H(11A)	1763	5801	3981	27
H(11B)	2338	6653	3335	27
H(12)	3956	6857	4749	19
H(14)	1855	6945	5935	22
H(15A)	-1072	6110	4655	45
H(15B)	65	6879	4584	45
H(15C)	-788	6737	5757	45
H(16A)	592	6718	7563	32

H(16B)	1071	5723	7673	32
H(17A)	2305	6513	9121	36
H(17B)	2848	7189	8172	36
H(19A)	4570	6138	9927	33
H(19B)	5894	5971	9107	33
H(20A)	6061	8149	10048	65
H(20B)	6851	7237	10232	65
H(20C)	5347	7403	10805	65
H(21A)	4567	4737	8428	29
H(21B)	3055	4949	8957	29
H(22A)	2602	3564	8159	30
H(22B)	3880	3479	7280	30
H(23A)	1846	2636	6688	58
H(23B)	2302	3302	5693	58
H(23C)	974	3518	6481	58
H(24)	2882	4652	5439	18
H(25)	5388	4239	6257	20
H(26)	6400	5895	6046	22
H(27A)	7775	4349	7029	51
H(27B)	8548	4927	8031	51
H(27C)	8367	5292	6719	51
H(27D)	8453	5438	7049	61
H(27E)	8362	5260	8427	61
H(27F)	7938	6191	7901	61
H(28)	4792	6812	6818	21
H(31A)	9509	3441	4414	52
H(31B)	9569	4444	4771	52
H(31C)	9105	4169	3458	52
H(32)	5990	6153	4410	18
H(33A)	5177	3934	3277	23
H(33B)	4197	3718	4351	23
H(34)	2347	4468	3616	25
H(35A)	2050	2967	1518	56
H(35B)	1426	3346	2700	56
H(35C)	2927	2854	2738	56

Table 94. Torsion angles [°] for e17phar1.

C(1)-O(1)-C(2)-C(7)	3.6(3)
C(1)-O(1)-C(2)-C(3)	-176.3(2)
O(1)-C(2)-C(3)-C(4)	-179.7(2)
C(7)-C(2)-C(3)-C(4)	0.4(3)
C(2)-C(3)-C(4)-C(5)	-0.5(3)
C(3)-C(4)-C(5)-C(6)	0.5(3)
C(3)-C(4)-C(5)-C(8)	179.8(2)
C(4)-C(5)-C(6)-C(7)	-0.3(3)
C(8)-C(5)-C(6)-C(7)	-179.61(19)
O(1)-C(2)-C(7)-C(6)	179.8(2)
C(3)-C(2)-C(7)-C(6)	-0.3(3)
C(5)-C(6)-C(7)-C(2)	0.2(3)
C(9)-O(3)-C(8)-O(2)	-0.4(3)
C(9)-O(3)-C(8)-C(5)	179.64(14)
C(6)-C(5)-C(8)-O(2)	-178.2(2)
C(4)-C(5)-C(8)-O(2)	2.5(3)
C(6)-C(5)-C(8)-O(3)	1.8(2)
C(4)-C(5)-C(8)-O(3)	-177.50(17)
C(8)-O(3)-C(9)-C(10)	170.51(15)
C(8)-O(3)-C(9)-C(32)	-76.1(2)
O(3)-C(9)-C(10)-O(4)	-69.48(19)
C(32)-C(9)-C(10)-O(4)	167.64(15)
O(3)-C(9)-C(10)-C(11)	172.83(14)
C(32)-C(9)-C(10)-C(11)	49.95(16)
O(3)-C(9)-C(10)-C(34)	56.16(18)
C(32)-C(9)-C(10)-C(34)	-66.71(17)
O(4)-C(10)-C(11)-C(12)	-155.24(15)
C(9)-C(10)-C(11)-C(12)	-35.28(18)
C(34)-C(10)-C(11)-C(12)	82.21(18)
C(10)-C(11)-C(12)-C(32)	7.31(18)
C(10)-C(11)-C(12)-C(13)	-122.74(16)
C(11)-C(12)-C(13)-C(24)	78.29(18)
C(32)-C(12)-C(13)-C(24)	-44.20(19)
C(11)-C(12)-C(13)-C(14)	-49.43(19)
C(32)-C(12)-C(13)-C(14)	-171.93(14)
C(11)-C(12)-C(13)-C(28)	-174.01(14)
C(32)-C(12)-C(13)-C(28)	63.49(19)

C(15)-O(5)-C(14)-C(16)	90.84(18)
C(15)-O(5)-C(14)-C(13)	-142.37(16)
C(24)-C(13)-C(14)-O(5)	-50.74(19)
C(28)-C(13)-C(14)-O(5)	-163.31(14)
C(12)-C(13)-C(14)-O(5)	73.82(17)
C(24)-C(13)-C(14)-C(16)	70.1(2)
C(28)-C(13)-C(14)-C(16)	-42.5(2)
C(12)-C(13)-C(14)-C(16)	-165.36(15)
O(5)-C(14)-C(16)-C(17)	166.69(17)
C(13)-C(14)-C(16)-C(17)	43.4(2)
C(14)-C(16)-C(17)-C(18)	-54.5(2)
C(16)-C(17)-C(18)-C(19)	-172.39(17)
C(16)-C(17)-C(18)-C(21)	-55.4(2)
C(16)-C(17)-C(18)-C(28)	64.6(2)
C(20)-O(6)-C(19)-C(18)	168.25(19)
C(17)-C(18)-C(19)-O(6)	-57.3(2)
C(21)-C(18)-C(19)-O(6)	-177.42(16)
C(28)-C(18)-C(19)-O(6)	62.1(2)
C(22)-N-C(21)-C(18)	171.16(16)
C(24)-N-C(21)-C(18)	41.5(2)
C(17)-C(18)-C(21)-N	77.0(2)
C(19)-C(18)-C(21)-N	-167.51(16)
C(28)-C(18)-C(21)-N	-43.3(2)
C(24)-N-C(22)-C(23)	-61.9(2)
C(21)-N-C(22)-C(23)	167.38(19)
C(22)-N-C(24)-C(13)	175.20(14)
C(21)-N-C(24)-C(13)	-57.2(2)
C(22)-N-C(24)-C(25)	-70.98(19)
C(21)-N-C(24)-C(25)	56.7(2)
C(14)-C(13)-C(24)-N	-51.96(19)
C(28)-C(13)-C(24)-N	69.06(16)
C(12)-C(13)-C(24)-N	-175.36(13)
C(14)-C(13)-C(24)-C(25)	-174.67(14)
C(28)-C(13)-C(24)-C(25)	-53.65(14)
C(12)-C(13)-C(24)-C(25)	61.93(16)
N-C(24)-C(25)-C(29)	162.08(14)
C(13)-C(24)-C(25)-C(29)	-78.17(16)
N-C(24)-C(25)-C(26)	-79.82(17)
C(13)-C(24)-C(25)-C(26)	39.93(15)

C(27A)-O(7)-C(26)-C(25)	128.5(8)
C(27)-O(7)-C(26)-C(25)	75.8(2)
C(27A)-O(7)-C(26)-C(28)	-112.5(8)
C(27)-O(7)-C(26)-C(28)	-165.2(2)
C(29)-C(25)-C(26)-O(7)	-129.01(15)
C(24)-C(25)-C(26)-O(7)	113.58(15)
C(29)-C(25)-C(26)-C(28)	107.53(15)
C(24)-C(25)-C(26)-C(28)	-9.88(16)
C(17)-C(18)-C(28)-C(26)	-172.98(15)
C(19)-C(18)-C(28)-C(26)	69.6(2)
C(21)-C(18)-C(28)-C(26)	-50.50(19)
C(17)-C(18)-C(28)-C(13)	-60.10(19)
C(19)-C(18)-C(28)-C(13)	-177.48(16)
C(21)-C(18)-C(28)-C(13)	62.38(18)
O(7)-C(26)-C(28)-C(18)	-29.2(2)
C(25)-C(26)-C(28)-C(18)	93.97(16)
O(7)-C(26)-C(28)-C(13)	-146.10(15)
C(25)-C(26)-C(28)-C(13)	-22.90(16)
C(24)-C(13)-C(28)-C(18)	-73.03(16)
C(14)-C(13)-C(28)-C(18)	49.84(19)
C(12)-C(13)-C(28)-C(18)	171.43(14)
C(24)-C(13)-C(28)-C(26)	47.23(15)
C(14)-C(13)-C(28)-C(26)	170.10(14)
C(12)-C(13)-C(28)-C(26)	-68.31(16)
C(30)-O(8)-C(29)-C(25)	69.2(2)
C(30)-O(8)-C(29)-C(32)	-175.82(15)
C(30)-O(8)-C(29)-C(33)	-56.8(2)
C(24)-C(25)-C(29)-O(8)	179.23(13)
C(26)-C(25)-C(29)-O(8)	65.40(17)
C(24)-C(25)-C(29)-C(32)	69.08(17)
C(26)-C(25)-C(29)-C(32)	-44.76(17)
C(24)-C(25)-C(29)-C(33)	-57.81(18)
C(26)-C(25)-C(29)-C(33)	-171.65(14)
C(29)-O(8)-C(30)-O(9)	-3.8(3)
C(29)-O(8)-C(30)-C(31)	175.37(16)
O(3)-C(9)-C(32)-C(29)	-42.71(19)
C(10)-C(9)-C(32)-C(29)	74.90(16)
O(3)-C(9)-C(32)-C(12)	-163.45(14)
C(10)-C(9)-C(32)-C(12)	-45.84(16)

O(8)-C(29)-C(32)-C(9)	86.63(15)
C(25)-C(29)-C(32)-C(9)	-157.41(13)
C(33)-C(29)-C(32)-C(9)	-29.62(19)
O(8)-C(29)-C(32)-C(12)	-158.40(13)
C(25)-C(29)-C(32)-C(12)	-42.44(18)
C(33)-C(29)-C(32)-C(12)	85.36(17)
C(11)-C(12)-C(32)-C(9)	23.20(16)
C(13)-C(12)-C(32)-C(9)	152.43(14)
C(11)-C(12)-C(32)-C(29)	-96.79(16)
C(13)-C(12)-C(32)-C(29)	32.4(2)
O(8)-C(29)-C(33)-C(34)	-134.41(15)
C(25)-C(29)-C(33)-C(34)	102.00(17)
C(32)-C(29)-C(33)-C(34)	-22.8(2)
C(35)-O(10)-C(34)-C(33)	80.5(2)
C(35)-O(10)-C(34)-C(10)	-154.25(17)
C(29)-C(33)-C(34)-O(10)	150.52(15)
C(29)-C(33)-C(34)-C(10)	29.4(2)
O(4)-C(10)-C(34)-O(10)	22.7(2)
C(9)-C(10)-C(34)-O(10)	-104.29(17)
C(11)-C(10)-C(34)-O(10)	144.93(14)
O(4)-C(10)-C(34)-C(33)	144.36(15)
C(9)-C(10)-C(34)-C(33)	17.3(2)
C(11)-C(10)-C(34)-C(33)	-93.45(18)

Table 95. Hydrogen bonds for e17phar1 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(4)-H(4A)...O(10)	0.80(3)	1.97(3)	2.562(2)	130(3)

s18phar2: aconitine hydrochloride trihydrate (**30b**)

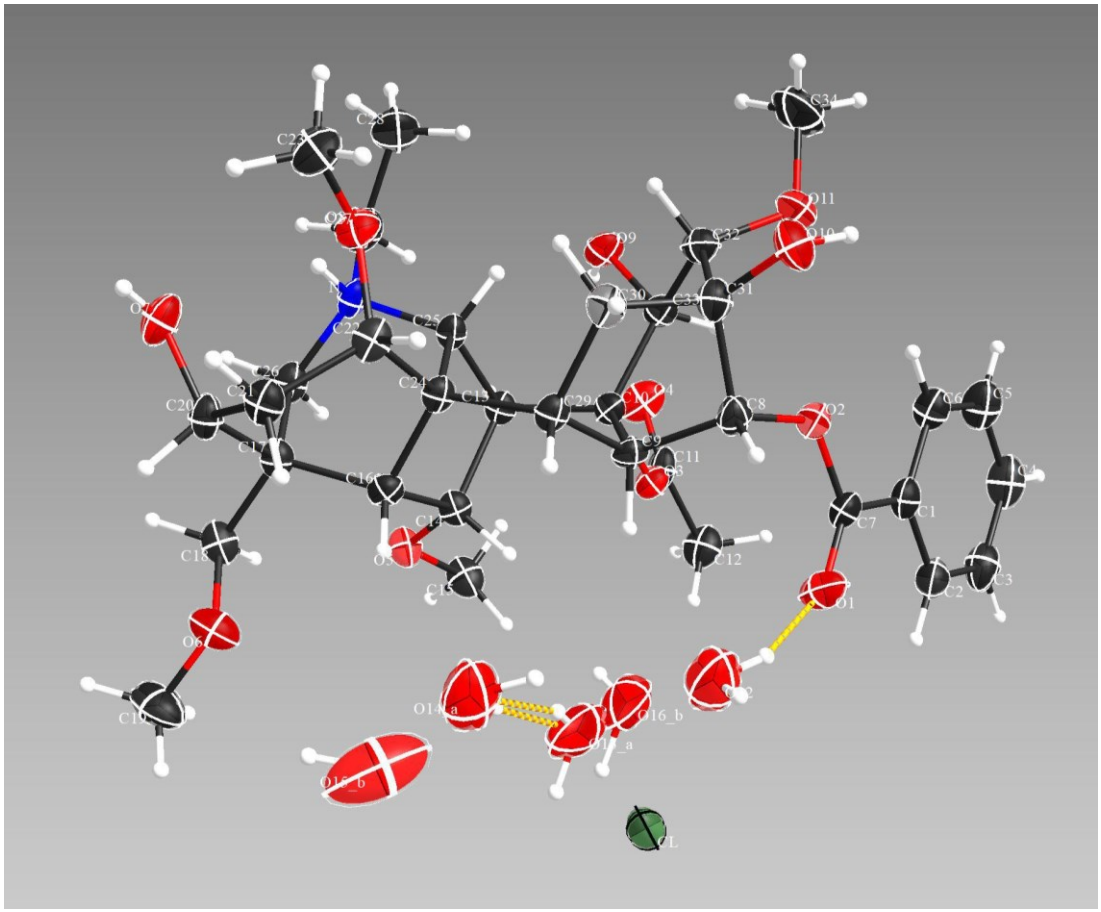

Table 96. Crystal data and structure refinement for s18phar2.

Identification code	s18phar2	
Empirical formula	C34 H54 Cl N O14	
Formula weight	736.23	
Temperature	150.00(10) K	
Wavelength	1.54184 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 12.7207(2) Å	α= 90°.
	b = 14.6595(2) Å	β= 90°.
	c = 19.2402(5) Å	γ = 90°.
Volume	3587.90(12) $Å^3$	
Z	4	
Density (calculated)	1.363 Mg/m^3	
Absorption coefficient	1.534 mm^{-1}	

F(000)	1576
Crystal size	0.320 x 0.090 x 0.030 mm^3
Theta range for data collection	3.791 to 73.181°.
Index ranges	-15<=h<=15, -12<=k<=17, -23<=l<=22
Reflections collected	26019
Independent reflections	7096 [R(int) = 0.0549]
Completeness to theta = 67.684°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.78728
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7096 / 18 / 511
Goodness-of-fit on F^2	1.045
Final R indices [I>2sigma(I)]	R1 = 0.0443, wR2 = 0.1020
R indices (all data)	R1 = 0.0523, wR2 = 0.1065
Absolute structure parameter	0.005(13)
Extinction coefficient	n/a
Largest diff. peak and hole	0.516 and -0.524 e.$Å^{-3}$

Table 97. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for s18phar2. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4070(3)	-87(2)	3516(2)	27(1)
C(2)	4263(3)	-459(3)	4171(2)	31(1)
C(3)	3953(3)	-1347(3)	4309(2)	36(1)
C(4)	3463(3)	-1860(3)	3795(2)	39(1)
C(5)	3269(3)	-1489(3)	3150(3)	39(1)
C(6)	3572(3)	-605(3)	3004(2)	32(1)
C(7)	4399(3)	867(2)	3374(2)	25(1)
C(8)	4165(2)	2096(2)	2577(2)	23(1)
C(9)	3449(2)	2731(2)	2987(2)	20(1)
C(10)	2307(3)	2373(2)	3024(2)	19(1)
C(11)	1566(3)	1267(2)	3862(2)	26(1)
C(12)	1818(3)	805(3)	4537(2)	35(1)
C(13)	1557(2)	3184(2)	3137(2)	19(1)
C(14)	2000(2)	3807(2)	3730(2)	21(1)

C(15)	1077(3)	3231(3)	4700(2)	31(1)
C(16)	2368(2)	4688(2)	3351(2)	20(1)
C(17)	1490(3)	5422(2)	3289(2)	22(1)
C(18)	1199(3)	5881(2)	3980(2)	29(1)
C(19)	1901(4)	6694(3)	4914(2)	48(1)
C(20)	1829(3)	6205(2)	2784(2)	25(1)
C(21)	2857(3)	6019(2)	2409(2)	24(1)
C(22)	2883(3)	5079(2)	2073(2)	23(1)
C(23)	2482(4)	5472(3)	894(2)	38(1)
C(24)	2619(2)	4318(2)	2608(2)	18(1)
C(25)	1605(2)	3774(2)	2474(2)	18(1)
C(26)	475(3)	4947(2)	3044(2)	23(1)
C(27)	-311(3)	3946(3)	2142(2)	31(1)
C(28)	-233(3)	3676(3)	1384(2)	42(1)
C(29)	3534(2)	3618(2)	2562(2)	20(1)
C(30)	3717(3)	3273(2)	1802(2)	24(1)
C(31)	3788(3)	2224(2)	1837(2)	25(1)
C(32)	2695(3)	1777(2)	1744(2)	25(1)
C(33)	2003(2)	1738(2)	2404(2)	22(1)
C(34)	2265(4)	601(3)	938(3)	53(1)
N	679(2)	4412(2)	2394(2)	21(1)
O(1)	4912(2)	1341(2)	3765(2)	37(1)
O(2)	4061(2)	1144(2)	2752(1)	25(1)
O(3)	2354(2)	1828(2)	3670(1)	22(1)
O(4)	779(2)	1144(2)	3529(2)	37(1)
O(5)	1263(2)	3999(2)	4265(1)	26(1)
O(6)	2134(2)	6224(2)	4291(1)	36(1)
O(7)	998(2)	6354(2)	2294(2)	32(1)
O(8)	2183(2)	4971(2)	1496(1)	27(1)
O(9)	957(2)	1869(2)	2164(1)	27(1)
O(10)	4487(2)	1913(2)	1321(2)	34(1)
O(11)	2839(2)	856(2)	1520(1)	36(1)
Cl	3451(1)	2089(1)	6267(1)	54(1)
O(12)	5984(3)	3126(3)	3759(3)	66(1)
O(13)	4176(5)	3410(6)	4824(3)	78(2)
O(14)	5031(4)	4935(4)	3923(4)	67(2)
O(15)	4536(18)	5550(20)	4563(12)	112(11)
O(16)	3790(20)	2680(20)	4877(10)	108(12)

Table 98. Bond lengths [Å] for s18phar2.

C(1)-C(2)	1.395(5)
C(1)-C(6)	1.395(5)
C(1)-C(7)	1.485(5)
C(2)-C(3)	1.385(6)
C(2)-H(2)	0.9500
C(3)-C(4)	1.390(6)
C(3)-H(3)	0.9500
C(4)-C(5)	1.377(6)
C(4)-H(4)	0.9500
C(5)-C(6)	1.381(6)
C(5)-H(5)	0.9500
C(6)-H(6)	0.9500
C(7)-O(1)	1.214(5)
C(7)-O(2)	1.335(4)
C(8)-O(2)	1.442(4)
C(8)-C(31)	1.514(5)
C(8)-C(9)	1.523(4)
C(8)-H(8)	1.0000
C(9)-C(29)	1.540(4)
C(9)-C(10)	1.546(4)
C(9)-H(9)	1.0000
C(10)-O(3)	1.480(4)
C(10)-C(13)	1.539(4)
C(10)-C(33)	1.562(4)
C(11)-O(4)	1.202(5)
C(11)-O(3)	1.348(4)
C(11)-C(12)	1.500(5)
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(25)	1.543(4)
C(13)-C(14)	1.567(4)
C(13)-H(13)	1.0000
C(14)-O(5)	1.420(4)
C(14)-C(16)	1.555(4)
C(14)-H(14)	1.0000
C(15)-O(5)	1.423(4)

C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(15)-H(15F)	0.9800
C(15)-H(15G)	0.9800
C(15)-H(15H)	0.9800
C(16)-C(17)	1.556(4)
C(16)-C(24)	1.562(4)
C(16)-H(16)	1.0000
C(17)-C(18)	1.535(5)
C(17)-C(26)	1.542(4)
C(17)-C(20)	1.565(5)
C(18)-O(6)	1.423(5)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-O(6)	1.414(5)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-O(7)	1.433(4)
C(20)-C(21)	1.518(5)
C(20)-H(20)	1.0000
C(21)-C(22)	1.523(5)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-O(8)	1.431(4)
C(22)-C(24)	1.555(4)
C(22)-H(22)	1.0000
C(23)-O(8)	1.423(4)
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-C(25)	1.539(4)
C(24)-C(29)	1.554(4)
C(25)-N	1.512(4)
C(25)-H(25)	1.0000
C(26)-N	1.499(5)
C(26)-H(26A)	0.9900
C(26)-H(26B)	0.9900

C(27)-N	1.512(4)
C(27)-C(28)	1.514(6)
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-C(30)	1.567(4)
C(29)-H(29)	1.0000
C(30)-C(31)	1.542(5)
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900
C(31)-O(10)	1.409(4)
C(31)-C(32)	1.547(5)
C(32)-O(11)	1.430(4)
C(32)-C(33)	1.546(5)
C(32)-H(32)	1.0000
C(33)-O(9)	1.421(4)
C(33)-H(33)	1.0000
C(34)-O(11)	1.388(5)
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
N-H	0.94(4)
O(7)-H(7)	0.87(3)
O(9)-H(9A)	0.87(3)
O(10)-H(10)	0.87(3)
O(12)-H(12D)	0.85(3)
O(12)-H(12E)	0.85(3)
O(13)-H(13A)	0.92(3)
O(13)-H(13B)	0.86(3)
O(14)-H(14A)	0.90(3)
O(14)-H(14B)	0.87(3)
O(15)-H(15D)	0.8680
O(15)-H(15E)	0.8638
O(16)-H(16B)	1.0116
O(16)-H(16A)	0.6025
O(16)-H(16B)	1.0116

Table 99. Bond angles [°] for s18phar2.

C(2)-C(1)-C(6)	120.3(3)
C(2)-C(1)-C(7)	118.9(3)
C(6)-C(1)-C(7)	120.7(3)
C(3)-C(2)-C(1)	119.3(4)
C(3)-C(2)-H(2)	120.3
C(1)-C(2)-H(2)	120.3
C(2)-C(3)-C(4)	120.1(4)
C(2)-C(3)-H(3)	120.0
C(4)-C(3)-H(3)	120.0
C(5)-C(4)-C(3)	120.4(4)
C(5)-C(4)-H(4)	119.8
C(3)-C(4)-H(4)	119.8
C(4)-C(5)-C(6)	120.4(4)
C(4)-C(5)-H(5)	119.8
C(6)-C(5)-H(5)	119.8
C(5)-C(6)-C(1)	119.5(4)
C(5)-C(6)-H(6)	120.2
C(1)-C(6)-H(6)	120.2
O(1)-C(7)-O(2)	123.6(3)
O(1)-C(7)-C(1)	125.3(3)
O(2)-C(7)-C(1)	111.1(3)
O(2)-C(8)-C(31)	108.1(3)
O(2)-C(8)-C(9)	114.5(3)
C(31)-C(8)-C(9)	102.8(3)
O(2)-C(8)-H(8)	110.4
C(31)-C(8)-H(8)	110.4
C(9)-C(8)-H(8)	110.4
C(8)-C(9)-C(29)	101.5(3)
C(8)-C(9)-C(10)	112.2(3)
C(29)-C(9)-C(10)	112.1(3)
C(8)-C(9)-H(9)	110.2
C(29)-C(9)-H(9)	110.2
C(10)-C(9)-H(9)	110.2
O(3)-C(10)-C(13)	108.8(3)
O(3)-C(10)-C(9)	100.6(2)
C(13)-C(10)-C(9)	109.1(2)
O(3)-C(10)-C(33)	109.3(2)

C(13)-C(10)-C(33)	114.5(3)
C(9)-C(10)-C(33)	113.6(3)
O(4)-C(11)-O(3)	124.4(3)
O(4)-C(11)-C(12)	124.9(3)
O(3)-C(11)-C(12)	110.7(3)
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(10)-C(13)-C(25)	106.9(3)
C(10)-C(13)-C(14)	109.3(3)
C(25)-C(13)-C(14)	105.1(2)
C(10)-C(13)-H(13)	111.7
C(25)-C(13)-H(13)	111.7
C(14)-C(13)-H(13)	111.7
O(5)-C(14)-C(16)	112.0(3)
O(5)-C(14)-C(13)	114.0(3)
C(16)-C(14)-C(13)	104.5(3)
O(5)-C(14)-H(14)	108.7
C(16)-C(14)-H(14)	108.7
C(13)-C(14)-H(14)	108.7
O(5)-C(15)-H(15A)	109.5
O(5)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
O(5)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
O(5)-C(15)-H(15F)	109.5
O(5)-C(15)-H(15G)	109.5
H(15F)-C(15)-H(15G)	109.5
O(5)-C(15)-H(15H)	109.5
H(15F)-C(15)-H(15H)	109.5
H(15G)-C(15)-H(15H)	109.5
C(14)-C(16)-C(17)	113.2(3)
C(14)-C(16)-C(24)	101.7(2)
C(17)-C(16)-C(24)	108.5(3)
C(14)-C(16)-H(16)	111.0

C(17)-C(16)-H(16)	111.0
C(24)-C(16)-H(16)	111.0
C(18)-C(17)-C(26)	105.1(3)
C(18)-C(17)-C(16)	114.2(3)
C(26)-C(17)-C(16)	108.2(3)
C(18)-C(17)-C(20)	106.5(3)
C(26)-C(17)-C(20)	111.9(3)
C(16)-C(17)-C(20)	110.9(3)
O(6)-C(18)-C(17)	108.5(3)
O(6)-C(18)-H(18A)	110.0
C(17)-C(18)-H(18A)	110.0
O(6)-C(18)-H(18B)	110.0
C(17)-C(18)-H(18B)	110.0
H(18A)-C(18)-H(18B)	108.4
O(6)-C(19)-H(19A)	109.5
O(6)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
O(6)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
O(7)-C(20)-C(21)	110.5(3)
O(7)-C(20)-C(17)	108.5(3)
C(21)-C(20)-C(17)	113.6(3)
O(7)-C(20)-H(20)	108.0
C(21)-C(20)-H(20)	108.0
C(17)-C(20)-H(20)	108.0
C(20)-C(21)-C(22)	112.5(3)
C(20)-C(21)-H(21A)	109.1
C(22)-C(21)-H(21A)	109.1
C(20)-C(21)-H(21B)	109.1
C(22)-C(21)-H(21B)	109.1
H(21A)-C(21)-H(21B)	107.8
O(8)-C(22)-C(21)	114.6(3)
O(8)-C(22)-C(24)	107.4(3)
C(21)-C(22)-C(24)	111.3(3)
O(8)-C(22)-H(22)	107.8
C(21)-C(22)-H(22)	107.8
C(24)-C(22)-H(22)	107.8
O(8)-C(23)-H(23A)	109.5

O(8)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
O(8)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(25)-C(24)-C(29)	106.0(2)
C(25)-C(24)-C(22)	116.2(3)
C(29)-C(24)-C(22)	105.9(2)
C(25)-C(24)-C(16)	99.3(2)
C(29)-C(24)-C(16)	115.7(3)
C(22)-C(24)-C(16)	113.6(3)
N-C(25)-C(24)	110.5(2)
N-C(25)-C(13)	113.6(3)
C(24)-C(25)-C(13)	100.6(2)
N-C(25)-H(25)	110.6
C(24)-C(25)-H(25)	110.6
C(13)-C(25)-H(25)	110.6
N-C(26)-C(17)	110.3(3)
N-C(26)-H(26A)	109.6
C(17)-C(26)-H(26A)	109.6
N-C(26)-H(26B)	109.6
C(17)-C(26)-H(26B)	109.6
H(26A)-C(26)-H(26B)	108.1
N-C(27)-C(28)	111.9(3)
N-C(27)-H(27A)	109.2
C(28)-C(27)-H(27A)	109.2
N-C(27)-H(27B)	109.2
C(28)-C(27)-H(27B)	109.2
H(27A)-C(27)-H(27B)	107.9
C(27)-C(28)-H(28A)	109.5
C(27)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(27)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(9)-C(29)-C(24)	118.3(3)
C(9)-C(29)-C(30)	103.5(2)
C(24)-C(29)-C(30)	112.2(3)
C(9)-C(29)-H(29)	107.4

C(24)-C(29)-H(29)	107.4
C(30)-C(29)-H(29)	107.4
C(31)-C(30)-C(29)	106.8(3)
C(31)-C(30)-H(30A)	110.4
C(29)-C(30)-H(30A)	110.4
C(31)-C(30)-H(30B)	110.4
C(29)-C(30)-H(30B)	110.4
H(30A)-C(30)-H(30B)	108.6
O(10)-C(31)-C(8)	115.0(3)
O(10)-C(31)-C(30)	109.1(3)
C(8)-C(31)-C(30)	100.6(3)
O(10)-C(31)-C(32)	110.4(3)
C(8)-C(31)-C(32)	110.0(3)
C(30)-C(31)-C(32)	111.3(3)
O(11)-C(32)-C(33)	106.6(3)
O(11)-C(32)-C(31)	108.6(3)
C(33)-C(32)-C(31)	115.6(3)
O(11)-C(32)-H(32)	108.6
C(33)-C(32)-H(32)	108.6
C(31)-C(32)-H(32)	108.6
O(9)-C(33)-C(32)	105.2(3)
O(9)-C(33)-C(10)	113.5(3)
C(32)-C(33)-C(10)	117.6(3)
O(9)-C(33)-H(33)	106.6
C(32)-C(33)-H(33)	106.6
C(10)-C(33)-H(33)	106.6
O(11)-C(34)-H(34A)	109.5
O(11)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
O(11)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(26)-N-C(27)	111.1(3)
C(26)-N-C(25)	111.9(3)
C(27)-N-C(25)	113.7(2)
C(26)-N-H	105(2)
C(27)-N-H	109(2)
C(25)-N-H	105(2)
C(7)-O(2)-C(8)	118.3(3)

C(11)-O(3)-C(10)	122.0(3)
C(14)-O(5)-C(15)	112.3(3)
C(19)-O(6)-C(18)	110.7(3)
C(20)-O(7)-H(7)	108(3)
C(23)-O(8)-C(22)	114.1(3)
C(33)-O(9)-H(9A)	110(5)
C(31)-O(10)-H(10)	108(4)
C(34)-O(11)-C(32)	115.5(3)
H(12D)-O(12)-H(12E)	108(4)
H(13A)-O(13)-H(13B)	100(4)
H(14A)-O(14)-H(14B)	98(4)
H(15D)-O(15)-H(15E)	102.8
H(16B)-O(16)-H(16A)	108.0
H(16B)-O(16)-H(16B)	0.0
H(16A)-O(16)-H(16B)	108.0

Table 100. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for s18phar2. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	21(2)	26(2)	33(2)	0(1)	2(1)	6(1)
C(2)	31(2)	32(2)	31(2)	2(2)	2(2)	10(2)
C(3)	33(2)	37(2)	40(2)	9(2)	10(2)	8(2)
C(4)	30(2)	32(2)	55(3)	8(2)	13(2)	0(2)
C(5)	29(2)	33(2)	54(3)	1(2)	1(2)	-3(2)
C(6)	27(2)	29(2)	38(2)	2(2)	-2(2)	2(1)
C(7)	21(2)	28(2)	28(2)	0(1)	-4(1)	7(1)
C(8)	17(1)	23(2)	29(2)	-2(1)	-1(1)	1(1)
C(9)	14(1)	24(2)	21(2)	0(1)	-2(1)	-2(1)
C(10)	19(2)	16(1)	22(2)	2(1)	-2(1)	-3(1)
C(11)	24(2)	21(2)	35(2)	6(1)	6(2)	1(1)
C(12)	37(2)	33(2)	35(2)	11(2)	6(2)	0(2)
C(13)	17(1)	18(1)	23(2)	2(1)	1(1)	-2(1)
C(14)	18(1)	21(1)	24(2)	-1(1)	2(1)	-2(1)
C(15)	40(2)	27(2)	26(2)	3(1)	10(2)	-3(2)

C(16)	18(2)	22(2)	22(2)	1(1)	-1(1)	-2(1)
C(17)	18(2)	20(1)	27(2)	1(1)	2(1)	-1(1)
C(18)	30(2)	24(2)	32(2)	-2(1)	6(1)	0(1)
C(19)	71(3)	45(2)	28(2)	-8(2)	5(2)	-11(2)
C(20)	23(2)	18(1)	33(2)	2(1)	1(1)	-1(1)
C(21)	21(2)	20(2)	31(2)	4(1)	2(1)	-5(1)
C(22)	18(2)	25(2)	27(2)	5(1)	5(1)	-1(1)
C(23)	54(3)	32(2)	29(2)	11(2)	5(2)	-2(2)
C(24)	12(1)	19(1)	23(2)	1(1)	1(1)	-1(1)
C(25)	14(1)	16(1)	25(2)	0(1)	-1(1)	-1(1)
C(26)	17(2)	21(2)	31(2)	4(1)	4(1)	0(1)
C(27)	15(2)	31(2)	46(2)	3(2)	-8(2)	-4(1)
C(28)	35(2)	43(2)	47(3)	-6(2)	-16(2)	-1(2)
C(29)	14(1)	20(1)	25(2)	2(1)	0(1)	-1(1)
C(30)	21(2)	26(2)	24(2)	3(1)	6(1)	1(1)
C(31)	21(2)	26(2)	28(2)	0(1)	3(1)	2(1)
C(32)	27(2)	25(2)	22(2)	0(1)	-4(1)	-2(1)
C(33)	20(2)	20(1)	26(2)	1(1)	-4(1)	-2(1)
C(34)	48(3)	59(3)	52(3)	-31(2)	-11(2)	1(2)
N	14(1)	20(1)	31(2)	4(1)	-3(1)	0(1)
O(1)	41(2)	32(1)	39(2)	4(1)	-17(1)	-5(1)
O(2)	25(1)	23(1)	27(1)	0(1)	-4(1)	3(1)
O(3)	23(1)	22(1)	22(1)	5(1)	0(1)	-1(1)
O(4)	27(1)	41(2)	42(2)	11(1)	-2(1)	-10(1)
O(5)	29(1)	23(1)	26(1)	1(1)	8(1)	0(1)
O(6)	40(2)	38(1)	30(1)	-8(1)	4(1)	-9(1)
O(7)	22(1)	32(1)	42(2)	11(1)	1(1)	3(1)
O(8)	29(1)	27(1)	24(1)	6(1)	1(1)	-3(1)
O(9)	19(1)	29(1)	32(1)	1(1)	-7(1)	-5(1)
O(10)	32(1)	35(1)	33(1)	-6(1)	9(1)	5(1)
O(11)	49(2)	29(1)	31(1)	-9(1)	-10(1)	4(1)
Cl	43(1)	46(1)	72(1)	-26(1)	-14(1)	10(1)
O(12)	52(2)	48(2)	98(3)	-10(2)	-24(2)	5(2)
O(13)	53(3)	121(6)	59(4)	-11(4)	-13(3)	43(4)
O(14)	39(3)	56(3)	106(5)	-9(3)	-12(3)	5(2)
O(15)	74(14)	180(30)	82(16)	30(17)	-22(11)	-2(16)
O(16)	150(20)	130(20)	47(11)	-20(13)	-30(12)	100(20)

Table 101. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for s18phar2.

	x	y	z	U(eq)
H(2)	4604	-107	4519	38
H(3)	4075	-1604	4755	44
H(4)	3260	-2472	3890	47
H(5)	2926	-1843	2805	46
H(6)	3442	-351	2558	38
H(8)	4915	2294	2622	28
H(9)	3733	2826	3466	24
H(12A)	2099	194	4445	52
H(12B)	1177	754	4818	52
H(12C)	2342	1165	4791	52
H(13)	824	2976	3239	23
H(14)	2627	3502	3941	25
H(15A)	566	3394	5060	47
H(15B)	799	2727	4420	47
H(15C)	1737	3042	4919	47
H(15F)	566	3394	5060	47
H(15G)	799	2727	4420	47
H(15H)	1737	3042	4919	47
H(16)	3012	4946	3575	25
H(18A)	698	6385	3897	35
H(18B)	861	5432	4294	35
H(19A)	1494	7244	4807	72
H(19B)	2557	6866	5146	72
H(19C)	1490	6297	5221	72
H(20)	1917	6775	3063	30
H(21A)	3444	6069	2745	29
H(21B)	2963	6489	2046	29
H(22)	3615	4970	1901	28
H(23A)	2045	5284	500	57
H(23B)	3222	5353	788	57
H(23C)	2383	6126	980	57
H(25)	1683	3381	2052	22
H(26A)	217	4533	3413	28
H(26B)	-75	5410	2954	28

H(27A)	-916	4362	2205	37
H(27B)	-439	3394	2426	37
H(28A)	-920	3462	1221	63
H(28B)	285	3187	1332	63
H(28C)	-15	4206	1108	63
H(29)	4190	3937	2714	24
H(30A)	3126	3461	1498	28
H(30B)	4376	3531	1611	28
H(32)	2304	2116	1374	30
H(33)	2044	1098	2581	26
H(34A)	2570	885	524	80
H(34B)	1535	801	992	80
H(34C)	2286	-64	888	80
H	890(30)	4840(30)	2070(20)	22(10)
H(7)	1220(40)	6740(30)	1980(20)	43(13)
H(9A)	520(40)	1740(50)	2490(30)	90(20)
H(10)	4450(50)	1322(18)	1310(30)	61(17)
H(12D)	6600(30)	3250(40)	3620(40)	99
H(12E)	5890(50)	2550(20)	3720(40)	99
H(13A)	4460(90)	3790(70)	4490(40)	117
H(13B)	4390(90)	3690(70)	5190(30)	117
H(14A)	4710(70)	4540(50)	4210(50)	100
H(14B)	5440(70)	4550(50)	3710(50)	100
H(15D)	4114	5139	4729	169
H(15E)	4140	6027	4537	169
H(16A)	3342	2767	4797	162
H(16B)	3924	2958	5352	162

Table 102. Torsion angles [°] for s18phar2.

C(6)-C(1)-C(2)-C(3)	-0.2(5)
C(7)-C(1)-C(2)-C(3)	179.6(3)
C(1)-C(2)-C(3)-C(4)	0.6(6)
C(2)-C(3)-C(4)-C(5)	-0.9(6)
C(3)-C(4)-C(5)-C(6)	0.8(6)
C(4)-C(5)-C(6)-C(1)	-0.4(6)

C(2)-C(1)-C(6)-C(5)	0.1(5)
C(7)-C(1)-C(6)-C(5)	-179.7(3)
C(2)-C(1)-C(7)-O(1)	6.8(5)
C(6)-C(1)-C(7)-O(1)	-173.4(4)
C(2)-C(1)-C(7)-O(2)	-173.6(3)
C(6)-C(1)-C(7)-O(2)	6.2(5)
O(2)-C(8)-C(9)-C(29)	-166.1(3)
C(31)-C(8)-C(9)-C(29)	-49.1(3)
O(2)-C(8)-C(9)-C(10)	-46.2(4)
C(31)-C(8)-C(9)-C(10)	70.7(3)
C(8)-C(9)-C(10)-O(3)	90.8(3)
C(29)-C(9)-C(10)-O(3)	-155.8(2)
C(8)-C(9)-C(10)-C(13)	-154.9(3)
C(29)-C(9)-C(10)-C(13)	-41.4(4)
C(8)-C(9)-C(10)-C(33)	-25.8(4)
C(29)-C(9)-C(10)-C(33)	87.6(3)
O(3)-C(10)-C(13)-C(25)	175.4(2)
C(9)-C(10)-C(13)-C(25)	66.5(3)
C(33)-C(10)-C(13)-C(25)	-62.0(3)
O(3)-C(10)-C(13)-C(14)	62.1(3)
C(9)-C(10)-C(13)-C(14)	-46.8(3)
C(33)-C(10)-C(13)-C(14)	-175.3(3)
C(10)-C(13)-C(14)-O(5)	-127.9(3)
C(25)-C(13)-C(14)-O(5)	117.6(3)
C(10)-C(13)-C(14)-C(16)	109.5(3)
C(25)-C(13)-C(14)-C(16)	-5.0(3)
O(5)-C(14)-C(16)-C(17)	-34.4(4)
C(13)-C(14)-C(16)-C(17)	89.4(3)
O(5)-C(14)-C(16)-C(24)	-150.6(2)
C(13)-C(14)-C(16)-C(24)	-26.7(3)
C(14)-C(16)-C(17)-C(18)	70.7(4)
C(24)-C(16)-C(17)-C(18)	-177.2(3)
C(14)-C(16)-C(17)-C(26)	-45.9(4)
C(24)-C(16)-C(17)-C(26)	66.1(3)
C(14)-C(16)-C(17)-C(20)	-169.0(3)
C(24)-C(16)-C(17)-C(20)	-56.9(3)
C(26)-C(17)-C(18)-O(6)	171.7(3)
C(16)-C(17)-C(18)-O(6)	53.3(4)
C(20)-C(17)-C(18)-O(6)	-69.5(3)

C(18)-C(17)-C(20)-O(7)	-105.0(3)
C(26)-C(17)-C(20)-O(7)	9.3(4)
C(16)-C(17)-C(20)-O(7)	130.2(3)
C(18)-C(17)-C(20)-C(21)	131.6(3)
C(26)-C(17)-C(20)-C(21)	-114.0(3)
C(16)-C(17)-C(20)-C(21)	6.8(4)
O(7)-C(20)-C(21)-C(22)	-72.5(3)
C(17)-C(20)-C(21)-C(22)	49.7(4)
C(20)-C(21)-C(22)-O(8)	68.5(4)
C(20)-C(21)-C(22)-C(24)	-53.6(4)
O(8)-C(22)-C(24)-C(25)	-10.5(4)
C(21)-C(22)-C(24)-C(25)	115.6(3)
O(8)-C(22)-C(24)-C(29)	106.9(3)
C(21)-C(22)-C(24)-C(29)	-126.9(3)
O(8)-C(22)-C(24)-C(16)	-124.9(3)
C(21)-C(22)-C(24)-C(16)	1.2(4)
C(14)-C(16)-C(24)-C(25)	48.7(3)
C(17)-C(16)-C(24)-C(25)	-70.8(3)
C(14)-C(16)-C(24)-C(29)	-64.2(3)
C(17)-C(16)-C(24)-C(29)	176.2(2)
C(14)-C(16)-C(24)-C(22)	172.9(2)
C(17)-C(16)-C(24)-C(22)	53.3(3)
C(29)-C(24)-C(25)-N	-171.1(3)
C(22)-C(24)-C(25)-N	-53.7(4)
C(16)-C(24)-C(25)-N	68.6(3)
C(29)-C(24)-C(25)-C(13)	68.6(3)
C(22)-C(24)-C(25)-C(13)	-174.0(3)
C(16)-C(24)-C(25)-C(13)	-51.7(3)
C(10)-C(13)-C(25)-N	161.1(2)
C(14)-C(13)-C(25)-N	-82.8(3)
C(10)-C(13)-C(25)-C(24)	-80.8(3)
C(14)-C(13)-C(25)-C(24)	35.3(3)
C(18)-C(17)-C(26)-N	-175.8(3)
C(16)-C(17)-C(26)-N	-53.5(3)
C(20)-C(17)-C(26)-N	69.0(3)
C(8)-C(9)-C(29)-C(24)	155.8(3)
C(10)-C(9)-C(29)-C(24)	35.8(4)
C(8)-C(9)-C(29)-C(30)	31.0(3)
C(10)-C(9)-C(29)-C(30)	-89.0(3)

C(25)-C(24)-C(29)-C(9)	-50.4(4)
C(22)-C(24)-C(29)-C(9)	-174.5(3)
C(16)-C(24)-C(29)-C(9)	58.6(4)
C(25)-C(24)-C(29)-C(30)	70.0(3)
C(22)-C(24)-C(29)-C(30)	-54.1(3)
C(16)-C(24)-C(29)-C(30)	179.0(3)
C(9)-C(29)-C(30)-C(31)	-3.1(3)
C(24)-C(29)-C(30)-C(31)	-131.8(3)
O(2)-C(8)-C(31)-O(10)	-75.1(3)
C(9)-C(8)-C(31)-O(10)	163.4(3)
O(2)-C(8)-C(31)-C(30)	167.8(2)
C(9)-C(8)-C(31)-C(30)	46.3(3)
O(2)-C(8)-C(31)-C(32)	50.3(3)
C(9)-C(8)-C(31)-C(32)	-71.2(3)
C(29)-C(30)-C(31)-O(10)	-147.5(3)
C(29)-C(30)-C(31)-C(8)	-26.1(3)
C(29)-C(30)-C(31)-C(32)	90.4(3)
O(10)-C(31)-C(32)-O(11)	36.9(4)
C(8)-C(31)-C(32)-O(11)	-91.1(3)
C(30)-C(31)-C(32)-O(11)	158.3(3)
O(10)-C(31)-C(32)-C(33)	156.6(3)
C(8)-C(31)-C(32)-C(33)	28.6(4)
C(30)-C(31)-C(32)-C(33)	-82.0(4)
O(11)-C(32)-C(33)-O(9)	-94.7(3)
C(31)-C(32)-C(33)-O(9)	144.5(3)
O(11)-C(32)-C(33)-C(10)	137.9(3)
C(31)-C(32)-C(33)-C(10)	17.1(4)
O(3)-C(10)-C(33)-O(9)	106.9(3)
C(13)-C(10)-C(33)-O(9)	-15.4(4)
C(9)-C(10)-C(33)-O(9)	-141.7(3)
O(3)-C(10)-C(33)-C(32)	-129.7(3)
C(13)-C(10)-C(33)-C(32)	107.9(3)
C(9)-C(10)-C(33)-C(32)	-18.4(4)
C(17)-C(26)-N-C(27)	-179.6(3)
C(17)-C(26)-N-C(25)	52.2(3)
C(28)-C(27)-N-C(26)	160.7(3)
C(28)-C(27)-N-C(25)	-71.9(4)
C(24)-C(25)-N-C(26)	-62.8(3)
C(13)-C(25)-N-C(26)	49.4(3)

C(24)-C(25)-N-C(27)	170.3(3)
C(13)-C(25)-N-C(27)	-77.5(3)
O(1)-C(7)-O(2)-C(8)	-10.1(5)
C(1)-C(7)-O(2)-C(8)	170.3(3)
C(31)-C(8)-O(2)-C(7)	176.8(3)
C(9)-C(8)-O(2)-C(7)	-69.3(4)
O(4)-C(11)-O(3)-C(10)	1.5(5)
C(12)-C(11)-O(3)-C(10)	-179.8(3)
C(13)-C(10)-O(3)-C(11)	75.6(3)
C(9)-C(10)-O(3)-C(11)	-169.9(3)
C(33)-C(10)-O(3)-C(11)	-50.1(4)
C(16)-C(14)-O(5)-C(15)	-168.6(3)
C(13)-C(14)-O(5)-C(15)	73.0(4)
C(17)-C(18)-O(6)-C(19)	177.1(3)
C(21)-C(22)-O(8)-C(23)	69.9(4)
C(24)-C(22)-O(8)-C(23)	-165.9(3)
C(33)-C(32)-O(11)-C(34)	105.4(4)
C(31)-C(32)-O(11)-C(34)	-129.4(4)

Table 103. Hydrogen bonds for s18phar2 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N-H...O(7)	0.94(4)	2.26(4)	2.882(4)	123(3)
N-H...O(8)	0.94(4)	1.98(4)	2.705(4)	133(3)
O(7)-H(7)...Cl#1	0.87(3)	2.24(3)	3.099(3)	169(5)
O(9)-H(9A)...O(4)	0.87(3)	2.20(6)	2.842(4)	130(6)
O(9)-H(9A)...O(7)#2	0.87(3)	2.05(5)	2.800(4)	145(6)
O(10)-H(10)...O(14^a)#3	0.87(3)	2.18(3)	3.001(6)	157(5)
O(10)-H(10)...O(15^b)#3	0.87(3)	2.39(6)	2.90(3)	118(5)
O(12)-H(12D)...Cl#4	0.85(3)	2.42(5)	3.155(4)	145(7)
O(12)-H(12E)...O(1)	0.85(3)	2.17(4)	2.951(5)	152(6)
O(13^a)-H(13A^a)...O(12)	0.92(3)	2.58(11)	3.108(8)	117(9)
O(13^a)-H(13A^a)...O(14^a)	0.92(3)	2.13(4)	3.030(11)	164(10)
O(14^a)-H(14A^a)...O(13^a)	0.90(3)	2.15(4)	3.030(11)	168(8)
O(14^a)-H(14B^a)...O(12)	0.87(3)	2.20(6)	2.932(6)	142(8)
O(15^b)-H(15E^b)...O(6)	0.86	2.61	3.25(2)	132.0
O(16^b)-H(16B^b)...Cl	1.01	2.26	2.85(2)	115.8

Symmetry transformations used to generate equivalent atoms:

#1 -x+1/2,-y+1,z-1/2 #2 -x,y-1/2,-z+1/2 #3 -x+1,y-1/2,-z+1/2

#4 x+1/2,-y+1/2,-z+1

e17phar3: lappaconitine hydrobrommide monohydrate (**20b**)

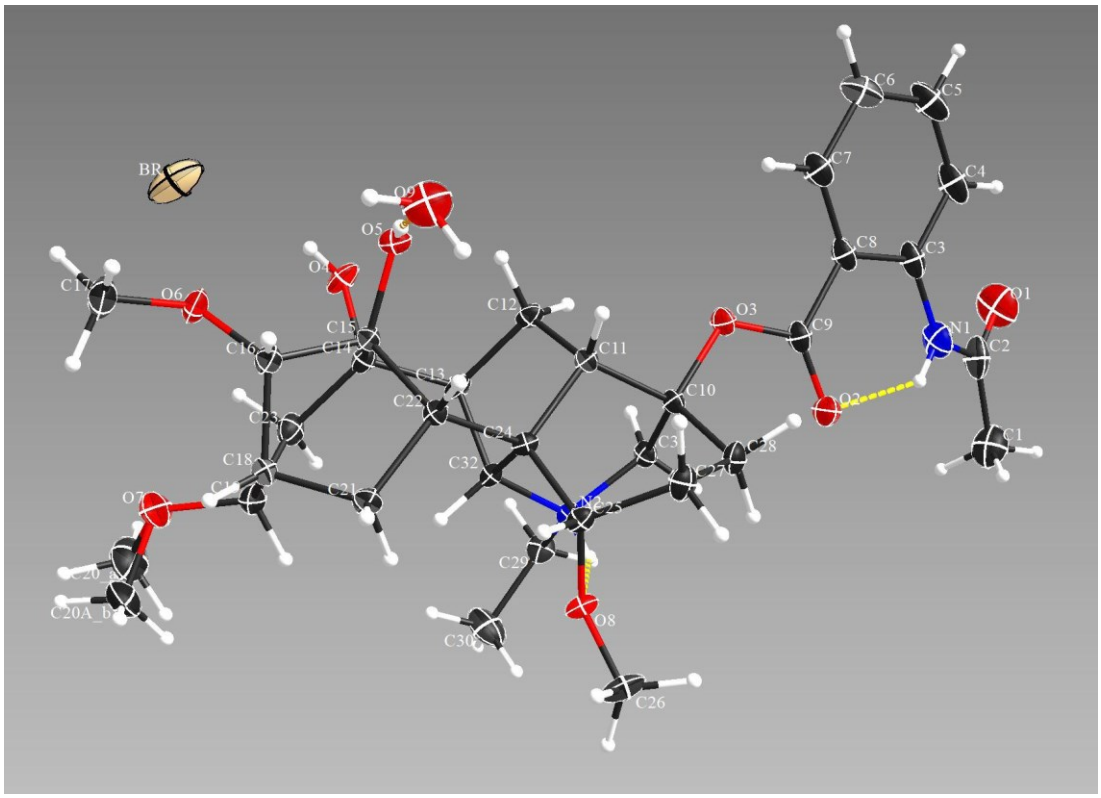

Table 104. Crystal data and structure refinement for e17phar3.

Identification code	e17phar3	
Empirical formula	C32 H47 Br N2 O9	
Formula weight	683.62	
Temperature	150.0(3) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 10.5121(2) Å	α= 90°.
	b = 12.16620(10) Å	β= 91.5660(10)°.
	c = 12.24300(10) Å	γ = 90°.
Volume	1565.20(3) $Å^3$	
Z	2	

Density (calculated)	1.451 Mg/m^3
Absorption coefficient	1.371 mm^{-1}
F(000)	720
Crystal size	0.500 x 0.300 x 0.200 mm^3
Theta range for data collection	3.329 to 30.400°.
Index ranges	-14<=h<=14, -17<=k<=17, -17<=l<=17
Reflections collected	108099
Independent reflections	8805 [R(int) = 0.0382]
Completeness to theta = 27.42°	99.76 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.83095
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8805 / 5 / 437
Goodness-of-fit on F^2	1.047
Final R indices [I>2sigma(I)]	R1 = 0.0309, wR2 = 0.0689
R indices (all data)	R1 = 0.0365, wR2 = 0.0709
Absolute structure parameter	-0.0086(17)
Extinction coefficient	n/a
Largest diff. peak and hole	0.675 and -0.329 $e.Å^{-3}$

Table 105. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for e17phar3. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	8909(3)	6405(3)	-2849(2)	36(1)
C(2)	9489(3)	7099(2)	-1952(2)	28(1)
C(3)	9700(2)	7122(2)	92(2)	22(1)
C(4)	10721(3)	7856(2)	199(2)	29(1)
C(5)	11114(3)	8244(2)	1211(3)	31(1)
C(6)	10507(3)	7925(2)	2151(2)	29(1)
C(7)	9486(2)	7200(2)	2058(2)	23(1)
C(8)	9077(2)	6788(2)	1047(2)	19(1)
C(9)	8020(2)	5978(2)	980(2)	18(1)
C(10)	6371(2)	5054(2)	1950(2)	14(1)
C(11)	5891(2)	5153(2)	3119(2)	13(1)
C(12)	5268(2)	6286(2)	3276(2)	15(1)

C(13)	3820(2)	6067(2)	3144(2)	14(1)
C(14)	3207(2)	6026(2)	4277(2)	15(1)
C(15)	3949(2)	5208(2)	5050(2)	14(1)
C(16)	3067(2)	4715(2)	5900(2)	16(1)
C(17)	1972(3)	5175(2)	7489(2)	28(1)
C(18)	2207(2)	3964(2)	5197(2)	18(1)
C(19)	1279(2)	4624(2)	4476(2)	23(1)
C(20)	-944(7)	4889(8)	4550(7)	40(2)
C(20A)	-770(5)	3962(5)	4790(5)	37(2)
C(21)	3210(2)	3366(2)	4515(2)	16(1)
C(22)	4361(2)	4166(2)	4427(2)	12(1)
C(23)	1758(2)	5776(2)	4199(2)	21(1)
C(24)	4792(2)	4307(2)	3234(2)	12(1)
C(25)	5129(2)	3135(2)	2833(2)	14(1)
C(26)	4434(3)	1761(2)	1543(2)	28(1)
C(27)	6530(2)	3062(2)	2573(2)	18(1)
C(28)	6905(2)	3898(2)	1717(2)	17(1)
C(29)	3028(2)	5460(2)	670(2)	19(1)
C(30)	1832(3)	4766(3)	621(2)	32(1)
C(31)	5323(2)	5438(2)	1137(2)	15(1)
C(32)	3740(2)	4932(2)	2600(2)	12(1)
N(1)	9312(2)	6686(2)	-923(2)	27(1)
N(2)	4048(2)	4949(2)	1393(2)	12(1)
O(1)	10068(2)	7950(2)	-2128(2)	41(1)
O(2)	7733(2)	5446(2)	165(1)	22(1)
O(3)	7404(2)	5874(1)	1918(1)	17(1)
O(4)	3340(2)	7131(1)	4687(1)	20(1)
O(5)	4984(2)	5770(1)	5566(1)	17(1)
O(6)	2475(2)	5564(1)	6494(1)	20(1)
O(7)	108(2)	4759(2)	5030(2)	42(1)
O(8)	4307(2)	2865(1)	1910(1)	17(1)
O(9)	6417(2)	4155(2)	6730(2)	31(1)
Br	4839(1)	3521(1)	8946(1)	30(1)

Table 106. Bond lengths [Å] for e17phar3.

C(1)-C(2)	1.502(4)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(2)-O(1)	1.223(4)
C(2)-N(1)	1.374(3)
C(3)-C(4)	1.400(4)
C(3)-N(1)	1.402(4)
C(3)-C(8)	1.416(3)
C(4)-C(5)	1.378(4)
C(4)-H(4)	0.9500
C(5)-C(6)	1.388(4)
C(5)-H(5)	0.9500
C(6)-C(7)	1.391(4)
C(6)-H(6)	0.9500
C(7)-C(8)	1.392(4)
C(7)-H(7)	0.9500
C(8)-C(9)	1.486(3)
C(9)-O(2)	1.220(3)
C(9)-O(3)	1.340(3)
C(10)-O(3)	1.476(2)
C(10)-C(11)	1.535(3)
C(10)-C(31)	1.537(3)
C(10)-C(28)	1.544(3)
C(11)-C(12)	1.541(3)
C(11)-C(24)	1.556(3)
C(11)-H(11)	1.0000
C(12)-C(13)	1.549(3)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(32)	1.536(3)
C(13)-C(14)	1.545(3)
C(13)-H(13)	1.0000
C(14)-O(4)	1.441(2)
C(14)-C(23)	1.554(3)
C(14)-C(15)	1.567(3)

C(15)-O(5)	1.418(3)
C(15)-C(16)	1.535(3)
C(15)-C(22)	1.548(3)
C(16)-O(6)	1.416(3)
C(16)-C(18)	1.533(3)
C(16)-H(16)	1.0000
C(17)-O(6)	1.422(3)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-C(19)	1.526(4)
C(18)-C(21)	1.545(3)
C(18)-H(18)	1.0000
C(19)-O(7)	1.431(3)
C(19)-C(23)	1.530(4)
C(19)-H(19)	1.0000
C(20)-O(7)	1.248(8)
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(20A)-O(7)	1.365(6)
C(20A)-H(20D)	0.9800
C(20A)-H(20E)	0.9800
C(20A)-H(20F)	0.9800
C(21)-C(22)	1.559(3)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-C(24)	1.550(3)
C(22)-H(22)	1.0000
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-C(32)	1.535(3)
C(24)-C(25)	1.553(3)
C(25)-O(8)	1.441(3)
C(25)-C(27)	1.517(3)
C(25)-H(25)	1.0000
C(26)-O(8)	1.424(3)
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800

C(26)-H(26C)	0.9800
C(27)-C(28)	1.520(3)
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(28)-H(28A)	0.9900
C(28)-H(28B)	0.9900
C(29)-N(2)	1.506(3)
C(29)-C(30)	1.514(4)
C(29)-H(29A)	0.9900
C(29)-H(29B)	0.9900
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-N(2)	1.507(3)
C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(32)-N(2)	1.521(3)
C(32)-H(32)	1.0000
N(1)-H(1)	0.81(4)
N(2)-H(2)	0.88(3)
O(4)-H(4A)	0.79(3)
O(5)-H(5A)	0.82(2)
O(9)-H(9A)	0.83(2)
O(9)-H(9B)	0.81(2)

Table 107. Bond angles [°] for e17phar3.

C(2)-C(1)-H(1A)	109.5
C(2)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
C(2)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
O(1)-C(2)-N(1)	123.5(3)
O(1)-C(2)-C(1)	122.8(3)
N(1)-C(2)-C(1)	113.7(3)

C(4)-C(3)-N(1)	121.9(2)
C(4)-C(3)-C(8)	118.5(2)
N(1)-C(3)-C(8)	119.6(2)
C(5)-C(4)-C(3)	120.8(2)
C(5)-C(4)-H(4)	119.6
C(3)-C(4)-H(4)	119.6
C(4)-C(5)-C(6)	121.1(2)
C(4)-C(5)-H(5)	119.4
C(6)-C(5)-H(5)	119.4
C(5)-C(6)-C(7)	118.7(3)
C(5)-C(6)-H(6)	120.6
C(7)-C(6)-H(6)	120.6
C(6)-C(7)-C(8)	121.3(2)
C(6)-C(7)-H(7)	119.3
C(8)-C(7)-H(7)	119.3
C(7)-C(8)-C(3)	119.5(2)
C(7)-C(8)-C(9)	120.1(2)
C(3)-C(8)-C(9)	120.4(2)
O(2)-C(9)-O(3)	122.5(2)
O(2)-C(9)-C(8)	124.4(2)
O(3)-C(9)-C(8)	113.1(2)
O(3)-C(10)-C(11)	103.45(16)
O(3)-C(10)-C(31)	107.00(16)
C(11)-C(10)-C(31)	109.38(17)
O(3)-C(10)-C(28)	109.84(17)
C(11)-C(10)-C(28)	111.99(17)
C(31)-C(10)-C(28)	114.50(18)
C(10)-C(11)-C(12)	109.79(17)
C(10)-C(11)-C(24)	107.24(16)
C(12)-C(11)-C(24)	105.15(17)
C(10)-C(11)-H(11)	111.5
C(12)-C(11)-H(11)	111.5
C(24)-C(11)-H(11)	111.5
C(11)-C(12)-C(13)	104.63(17)
C(11)-C(12)-H(12A)	110.8
C(13)-C(12)-H(12A)	110.8
C(11)-C(12)-H(12B)	110.8
C(13)-C(12)-H(12B)	110.8
H(12A)-C(12)-H(12B)	108.9

C(32)-C(13)-C(14)	109.95(16)
C(32)-C(13)-C(12)	104.03(17)
C(14)-C(13)-C(12)	110.17(17)
C(32)-C(13)-H(13)	110.8
C(14)-C(13)-H(13)	110.8
C(12)-C(13)-H(13)	110.8
O(4)-C(14)-C(13)	104.13(16)
O(4)-C(14)-C(23)	106.85(17)
C(13)-C(14)-C(23)	112.55(18)
O(4)-C(14)-C(15)	109.88(17)
C(13)-C(14)-C(15)	110.46(16)
C(23)-C(14)-C(15)	112.55(17)
O(5)-C(15)-C(16)	110.88(17)
O(5)-C(15)-C(22)	113.11(17)
C(16)-C(15)-C(22)	101.31(16)
O(5)-C(15)-C(14)	109.05(16)
C(16)-C(15)-C(14)	111.00(17)
C(22)-C(15)-C(14)	111.33(17)
O(6)-C(16)-C(18)	117.50(19)
O(6)-C(16)-C(15)	110.17(17)
C(18)-C(16)-C(15)	102.14(17)
O(6)-C(16)-H(16)	108.9
C(18)-C(16)-H(16)	108.9
C(15)-C(16)-H(16)	108.9
O(6)-C(17)-H(17A)	109.5
O(6)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
O(6)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(19)-C(18)-C(16)	111.65(19)
C(19)-C(18)-C(21)	111.67(19)
C(16)-C(18)-C(21)	100.59(18)
C(19)-C(18)-H(18)	110.8
C(16)-C(18)-H(18)	110.8
C(21)-C(18)-H(18)	110.8
O(7)-C(19)-C(18)	109.3(2)
O(7)-C(19)-C(23)	107.0(2)
C(18)-C(19)-C(23)	113.7(2)

O(7)-C(19)-H(19)	108.9
C(18)-C(19)-H(19)	108.9
C(23)-C(19)-H(19)	108.9
O(7)-C(20)-H(20A)	109.5
O(7)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
O(7)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
O(7)-C(20A)-H(20D)	109.5
O(7)-C(20A)-H(20E)	109.5
H(20D)-C(20A)-H(20E)	109.5
O(7)-C(20A)-H(20F)	109.5
H(20D)-C(20A)-H(20F)	109.5
H(20E)-C(20A)-H(20F)	109.5
C(18)-C(21)-C(22)	106.62(17)
C(18)-C(21)-H(21A)	110.4
C(22)-C(21)-H(21A)	110.4
C(18)-C(21)-H(21B)	110.4
C(22)-C(21)-H(21B)	110.4
H(21A)-C(21)-H(21B)	108.6
C(15)-C(22)-C(24)	117.80(16)
C(15)-C(22)-C(21)	104.41(16)
C(24)-C(22)-C(21)	112.44(17)
C(15)-C(22)-H(22)	107.2
C(24)-C(22)-H(22)	107.2
C(21)-C(22)-H(22)	107.2
C(19)-C(23)-C(14)	119.58(19)
C(19)-C(23)-H(23A)	107.4
C(14)-C(23)-H(23A)	107.4
C(19)-C(23)-H(23B)	107.4
C(14)-C(23)-H(23B)	107.4
H(23A)-C(23)-H(23B)	107.0
C(32)-C(24)-C(22)	107.85(16)
C(32)-C(24)-C(25)	117.52(17)
C(22)-C(24)-C(25)	105.74(16)
C(32)-C(24)-C(11)	98.81(16)
C(22)-C(24)-C(11)	113.30(17)
C(25)-C(24)-C(11)	113.72(17)

O(8)-C(25)-C(27)	112.78(18)
O(8)-C(25)-C(24)	108.67(17)
C(27)-C(25)-C(24)	110.57(18)
O(8)-C(25)-H(25)	108.2
C(27)-C(25)-H(25)	108.2
C(24)-C(25)-H(25)	108.2
O(8)-C(26)-H(26A)	109.5
O(8)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
O(8)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(25)-C(27)-C(28)	112.13(18)
C(25)-C(27)-H(27A)	109.2
C(28)-C(27)-H(27A)	109.2
C(25)-C(27)-H(27B)	109.2
C(28)-C(27)-H(27B)	109.2
H(27A)-C(27)-H(27B)	107.9
C(27)-C(28)-C(10)	112.30(18)
C(27)-C(28)-H(28A)	109.1
C(10)-C(28)-H(28A)	109.1
C(27)-C(28)-H(28B)	109.1
C(10)-C(28)-H(28B)	109.1
H(28A)-C(28)-H(28B)	107.9
N(2)-C(29)-C(30)	111.72(19)
N(2)-C(29)-H(29A)	109.3
C(30)-C(29)-H(29A)	109.3
N(2)-C(29)-H(29B)	109.3
C(30)-C(29)-H(29B)	109.3
H(29A)-C(29)-H(29B)	107.9
C(29)-C(30)-H(30A)	109.5
C(29)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(29)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
N(2)-C(31)-C(10)	111.80(16)
N(2)-C(31)-H(31A)	109.3
C(10)-C(31)-H(31A)	109.3

N(2)-C(31)-H(31B)	109.3
C(10)-C(31)-H(31B)	109.3
H(31A)-C(31)-H(31B)	107.9
N(2)-C(32)-C(24)	109.21(16)
N(2)-C(32)-C(13)	113.49(16)
C(24)-C(32)-C(13)	101.26(17)
N(2)-C(32)-H(32)	110.8
C(24)-C(32)-H(32)	110.8
C(13)-C(32)-H(32)	110.8
C(2)-N(1)-C(3)	129.2(2)
C(2)-N(1)-H(1)	115(3)
C(3)-N(1)-H(1)	115(3)
C(29)-N(2)-C(31)	109.75(16)
C(29)-N(2)-C(32)	114.20(17)
C(31)-N(2)-C(32)	114.93(16)
C(29)-N(2)-H(2)	110.5(18)
C(31)-N(2)-H(2)	103.1(18)
C(32)-N(2)-H(2)	103.6(19)
C(9)-O(3)-C(10)	117.36(17)
C(14)-O(4)-H(4A)	106(4)
C(15)-O(5)-H(5A)	109(3)
C(16)-O(6)-C(17)	112.10(18)
C(20)-O(7)-C(19)	123.6(4)
C(20A)-O(7)-C(19)	113.7(3)
C(26)-O(8)-C(25)	113.80(18)
H(9A)-O(9)-H(9B)	107(4)

Table 108. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for e17phar3. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	40(2)	43(2)	26(1)	6(1)	2(1)	8(1)
C(2)	25(1)	34(1)	27(1)	10(1)	10(1)	8(1)
C(3)	16(1)	22(1)	27(1)	8(1)	4(1)	2(1)
C(4)	20(1)	31(1)	36(1)	12(1)	6(1)	-4(1)

C(5)	21(1)	26(1)	46(2)	10(1)	-2(1)	-7(1)
C(6)	27(1)	24(1)	36(1)	2(1)	-7(1)	-6(1)
C(7)	21(1)	22(1)	26(1)	4(1)	2(1)	-3(1)
C(8)	15(1)	18(1)	24(1)	6(1)	3(1)	-1(1)
C(9)	16(1)	18(1)	20(1)	3(1)	3(1)	0(1)
C(10)	13(1)	14(1)	14(1)	0(1)	2(1)	-2(1)
C(11)	14(1)	12(1)	12(1)	0(1)	1(1)	-1(1)
C(12)	21(1)	11(1)	14(1)	-1(1)	2(1)	-2(1)
C(13)	20(1)	10(1)	12(1)	0(1)	1(1)	2(1)
C(14)	18(1)	12(1)	14(1)	-2(1)	2(1)	2(1)
C(15)	16(1)	13(1)	12(1)	-1(1)	2(1)	-1(1)
C(16)	19(1)	16(1)	13(1)	-1(1)	3(1)	-1(1)
C(17)	32(1)	32(1)	22(1)	-2(1)	13(1)	-1(1)
C(18)	19(1)	18(1)	17(1)	-2(1)	5(1)	-5(1)
C(19)	16(1)	30(1)	23(1)	-10(1)	4(1)	-1(1)
C(20)	22(4)	62(6)	36(4)	-4(3)	-2(3)	4(3)
C(20A)	22(3)	52(3)	37(3)	-6(2)	6(2)	-14(2)
C(21)	21(1)	12(1)	17(1)	0(1)	3(1)	-4(1)
C(22)	14(1)	12(1)	12(1)	0(1)	1(1)	0(1)
C(23)	16(1)	26(1)	19(1)	-2(1)	0(1)	5(1)
C(24)	14(1)	10(1)	11(1)	0(1)	-1(1)	1(1)
C(25)	18(1)	10(1)	13(1)	1(1)	1(1)	1(1)
C(26)	40(2)	15(1)	29(1)	-10(1)	-2(1)	2(1)
C(27)	19(1)	15(1)	20(1)	1(1)	2(1)	6(1)
C(28)	16(1)	17(1)	18(1)	-1(1)	4(1)	4(1)
C(29)	20(1)	22(1)	14(1)	3(1)	-3(1)	4(1)
C(30)	20(1)	45(2)	32(1)	10(1)	-8(1)	-4(1)
C(31)	16(1)	14(1)	14(1)	2(1)	3(1)	-1(1)
C(32)	15(1)	11(1)	10(1)	-1(1)	1(1)	1(1)
N(1)	27(1)	30(1)	24(1)	5(1)	7(1)	-4(1)
N(2)	14(1)	12(1)	11(1)	0(1)	1(1)	1(1)
O(1)	47(1)	43(1)	34(1)	16(1)	8(1)	-8(1)
O(2)	22(1)	27(1)	18(1)	-2(1)	4(1)	-5(1)
O(3)	16(1)	20(1)	16(1)	0(1)	4(1)	-5(1)
O(4)	32(1)	13(1)	16(1)	-4(1)	2(1)	4(1)
O(5)	20(1)	16(1)	14(1)	-1(1)	-2(1)	-2(1)
O(6)	25(1)	20(1)	15(1)	-3(1)	7(1)	1(1)
O(7)	16(1)	58(1)	52(1)	-28(1)	10(1)	-7(1)
O(8)	23(1)	12(1)	15(1)	-4(1)	-1(1)	0(1)

O(9)	37(1)	28(1)	28(1)	2(1)	-3(1)	2(1)
Br	50(1)	19(1)	22(1)	-6(1)	-2(1)	2(1)

Table 109. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for e17phar3.

	x	y	z	U(eq)
H(1A)	9366	6528	-3525	55
H(1B)	8013	6607	-2964	55
H(1C)	8969	5628	-2644	55
H(4)	11149	8090	-434	35
H(5)	11813	8738	1265	37
H(6)	10783	8196	2846	35
H(7)	9059	6982	2697	28
H(11)	6590	5021	3673	15
H(12A)	5554	6814	2718	18
H(12B)	5481	6585	4011	18
H(13)	3402	6639	2670	17
H(16)	3585	4252	6420	19
H(17A)	1650	5797	7908	43
H(17B)	2643	4800	7917	43
H(17C)	1275	4660	7327	43
H(18)	1742	3432	5664	22
H(19)	1109	4211	3781	27
H(20A)	-1037	5658	4325	60
H(20B)	-1627	4696	5044	60
H(20C)	-994	4414	3903	60
H(20D)	-874	3891	3995	55
H(20E)	-1587	4163	5101	55
H(20F)	-480	3260	5100	55
H(21A)	2854	3188	3779	20
H(21B)	3479	2674	4878	20
H(22)	5090	3833	4852	15
H(23A)	1328	6301	4684	25
H(23B)	1462	5943	3442	25

H(25)	4957	2604	3434	17
H(26A)	3721	1580	1042	42
H(26B)	4431	1262	2171	42
H(26C)	5236	1681	1162	42
H(27A)	6720	2313	2305	22
H(27B)	7046	3186	3250	22
H(28A)	6586	3650	990	20
H(28B)	7845	3938	1697	20
H(29A)	3352	5549	-76	22
H(29B)	2821	6200	953	22
H(30A)	1218	5089	96	49
H(30B)	1459	4742	1346	49
H(30C)	2044	4019	390	49
H(31A)	5263	6249	1160	17
H(31B)	5553	5222	388	17
H(32)	2890	4587	2714	14
H(1)	8830(30)	6160(30)	-890(30)	31(9)
H(2)	4140(30)	4250(30)	1230(20)	14(6)
H(4A)	3390(50)	7080(50)	5330(20)	81(16)
H(5A)	5390(30)	5330(30)	5950(30)	38(10)
H(9A)	6560(30)	3570(30)	6420(30)	46(10)
H(9B)	6050(30)	4000(30)	7280(20)	35(10)

Table 110. Torsion angles [°] for e17phar3.

N(1)-C(3)-C(4)-C(5)	-177.7(3)
C(8)-C(3)-C(4)-C(5)	0.2(4)
C(3)-C(4)-C(5)-C(6)	-0.4(4)
C(4)-C(5)-C(6)-C(7)	0.0(4)
C(5)-C(6)-C(7)-C(8)	0.6(4)
C(6)-C(7)-C(8)-C(3)	-0.8(4)
C(6)-C(7)-C(8)-C(9)	177.4(2)
C(4)-C(3)-C(8)-C(7)	0.4(3)
N(1)-C(3)-C(8)-C(7)	178.4(2)
C(4)-C(3)-C(8)-C(9)	-177.8(2)
N(1)-C(3)-C(8)-C(9)	0.2(3)

C(7)-C(8)-C(9)-O(2)	-167.9(2)
C(3)-C(8)-C(9)-O(2)	10.3(4)
C(7)-C(8)-C(9)-O(3)	11.4(3)
C(3)-C(8)-C(9)-O(3)	-170.4(2)
O(3)-C(10)-C(11)-C(12)	66.5(2)
C(31)-C(10)-C(11)-C(12)	-47.2(2)
C(28)-C(10)-C(11)-C(12)	-175.27(18)
O(3)-C(10)-C(11)-C(24)	-179.76(16)
C(31)-C(10)-C(11)-C(24)	66.5(2)
C(28)-C(10)-C(11)-C(24)	-61.5(2)
C(10)-C(11)-C(12)-C(13)	99.54(19)
C(24)-C(11)-C(12)-C(13)	-15.5(2)
C(11)-C(12)-C(13)-C(32)	-16.0(2)
C(11)-C(12)-C(13)-C(14)	101.79(19)
C(32)-C(13)-C(14)-O(4)	-179.66(17)
C(12)-C(13)-C(14)-O(4)	66.2(2)
C(32)-C(13)-C(14)-C(23)	-64.3(2)
C(12)-C(13)-C(14)-C(23)	-178.40(18)
C(32)-C(13)-C(14)-C(15)	62.4(2)
C(12)-C(13)-C(14)-C(15)	-51.7(2)
O(4)-C(14)-C(15)-O(5)	-28.5(2)
C(13)-C(14)-C(15)-O(5)	85.9(2)
C(23)-C(14)-C(15)-O(5)	-147.40(17)
O(4)-C(14)-C(15)-C(16)	94.0(2)
C(13)-C(14)-C(15)-C(16)	-151.68(17)
C(23)-C(14)-C(15)-C(16)	-25.0(2)
O(4)-C(14)-C(15)-C(22)	-153.96(17)
C(13)-C(14)-C(15)-C(22)	-39.6(2)
C(23)-C(14)-C(15)-C(22)	87.1(2)
O(5)-C(15)-C(16)-O(6)	65.8(2)
C(22)-C(15)-C(16)-O(6)	-173.91(18)
C(14)-C(15)-C(16)-O(6)	-55.6(2)
O(5)-C(15)-C(16)-C(18)	-168.62(18)
C(22)-C(15)-C(16)-C(18)	-48.3(2)
C(14)-C(15)-C(16)-C(18)	70.0(2)
O(6)-C(16)-C(18)-C(19)	49.1(3)
C(15)-C(16)-C(18)-C(19)	-71.5(2)
O(6)-C(16)-C(18)-C(21)	167.67(18)
C(15)-C(16)-C(18)-C(21)	47.0(2)

C(16)-C(18)-C(19)-O(7)	-93.0(2)
C(21)-C(18)-C(19)-O(7)	155.29(19)
C(16)-C(18)-C(19)-C(23)	26.5(3)
C(21)-C(18)-C(19)-C(23)	-85.3(2)
C(19)-C(18)-C(21)-C(22)	90.7(2)
C(16)-C(18)-C(21)-C(22)	-27.9(2)
O(5)-C(15)-C(22)-C(24)	-86.0(2)
C(16)-C(15)-C(22)-C(24)	155.31(18)
C(14)-C(15)-C(22)-C(24)	37.2(2)
O(5)-C(15)-C(22)-C(21)	148.51(17)
C(16)-C(15)-C(22)-C(21)	29.8(2)
C(14)-C(15)-C(22)-C(21)	-88.28(19)
C(18)-C(21)-C(22)-C(15)	-1.2(2)
C(18)-C(21)-C(22)-C(24)	-130.01(18)
O(7)-C(19)-C(23)-C(14)	142.4(2)
C(18)-C(19)-C(23)-C(14)	21.6(3)
O(4)-C(14)-C(23)-C(19)	-142.9(2)
C(13)-C(14)-C(23)-C(19)	103.4(2)
C(15)-C(14)-C(23)-C(19)	-22.2(3)
C(15)-C(22)-C(24)-C(32)	-53.0(2)
C(21)-C(22)-C(24)-C(32)	68.4(2)
C(15)-C(22)-C(24)-C(25)	-179.55(18)
C(21)-C(22)-C(24)-C(25)	-58.1(2)
C(15)-C(22)-C(24)-C(11)	55.3(2)
C(21)-C(22)-C(24)-C(11)	176.73(17)
C(10)-C(11)-C(24)-C(32)	-76.05(18)
C(12)-C(11)-C(24)-C(32)	40.77(19)
C(10)-C(11)-C(24)-C(22)	170.09(17)
C(12)-C(11)-C(24)-C(22)	-73.1(2)
C(10)-C(11)-C(24)-C(25)	49.3(2)
C(12)-C(11)-C(24)-C(25)	166.13(17)
C(32)-C(24)-C(25)-O(8)	-1.4(2)
C(22)-C(24)-C(25)-O(8)	118.95(18)
C(11)-C(24)-C(25)-O(8)	-116.11(19)
C(32)-C(24)-C(25)-C(27)	122.9(2)
C(22)-C(24)-C(25)-C(27)	-116.75(19)
C(11)-C(24)-C(25)-C(27)	8.2(2)
O(8)-C(25)-C(27)-C(28)	64.2(2)
C(24)-C(25)-C(27)-C(28)	-57.7(2)

C(25)-C(27)-C(28)-C(10)	46.0(3)
O(3)-C(10)-C(28)-C(27)	128.9(2)
C(11)-C(10)-C(28)-C(27)	14.6(3)
C(31)-C(10)-C(28)-C(27)	-110.7(2)
O(3)-C(10)-C(31)-N(2)	-157.90(16)
C(11)-C(10)-C(31)-N(2)	-46.5(2)
C(28)-C(10)-C(31)-N(2)	80.1(2)
C(22)-C(24)-C(32)-N(2)	-172.38(16)
C(25)-C(24)-C(32)-N(2)	-53.1(2)
C(11)-C(24)-C(32)-N(2)	69.57(18)
C(22)-C(24)-C(32)-C(13)	67.64(19)
C(25)-C(24)-C(32)-C(13)	-173.07(17)
C(11)-C(24)-C(32)-C(13)	-50.41(18)
C(14)-C(13)-C(32)-N(2)	167.16(17)
C(12)-C(13)-C(32)-N(2)	-74.9(2)
C(14)-C(13)-C(32)-C(24)	-75.9(2)
C(12)-C(13)-C(32)-C(24)	42.02(19)
O(1)-C(2)-N(1)-C(3)	1.3(4)
C(1)-C(2)-N(1)-C(3)	-178.9(2)
C(4)-C(3)-N(1)-C(2)	-23.4(4)
C(8)-C(3)-N(1)-C(2)	158.7(3)
C(30)-C(29)-N(2)-C(31)	161.4(2)
C(30)-C(29)-N(2)-C(32)	-67.9(3)
C(10)-C(31)-N(2)-C(29)	172.67(17)
C(10)-C(31)-N(2)-C(32)	42.3(2)
C(24)-C(32)-N(2)-C(29)	175.24(17)
C(13)-C(32)-N(2)-C(29)	-72.6(2)
C(24)-C(32)-N(2)-C(31)	-56.6(2)
C(13)-C(32)-N(2)-C(31)	55.5(2)
O(2)-C(9)-O(3)-C(10)	1.9(3)
C(8)-C(9)-O(3)-C(10)	-177.44(18)
C(11)-C(10)-O(3)-C(9)	179.91(18)
C(31)-C(10)-O(3)-C(9)	-64.6(2)
C(28)-C(10)-O(3)-C(9)	60.2(2)
C(18)-C(16)-O(6)-C(17)	81.7(3)
C(15)-C(16)-O(6)-C(17)	-162.0(2)
C(18)-C(19)-O(7)-C(20)	-153.0(6)
C(23)-C(19)-O(7)-C(20)	83.5(6)
C(18)-C(19)-O(7)-C(20A)	-92.4(4)

C(23)-C(19)-O(7)-C(20A)	144.1(4)
C(27)-C(25)-O(8)-C(26)	63.4(2)
C(24)-C(25)-O(8)-C(26)	-173.61(19)

Table 111. Hydrogen bonds for e17phar3 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1)...O(2)	0.81(4)	1.96(4)	2.632(3)	139(3)
N(2)-H(2)...O(8)	0.88(3)	1.88(3)	2.626(2)	141(3)
N(2)-H(2)...Br#1	0.88(3)	3.04(3)	3.5814(18)	121(2)
O(4)-H(4A)...O(6)	0.79(3)	2.54(5)	3.077(2)	127(5)
O(5)-H(5A)...O(9)	0.82(2)	2.02(2)	2.836(3)	173(4)
O(9)-H(9A)...O(4)#2	0.83(2)	2.21(3)	3.027(3)	168(4)
O(9)-H(9B)...Br	0.81(2)	2.50(2)	3.310(2)	178(3)

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z-1 #2 -x+1,y-1/2,-z+1

s17phar14: methyllycaconitine perchlorate monomethanol dihydrate (**31b**)

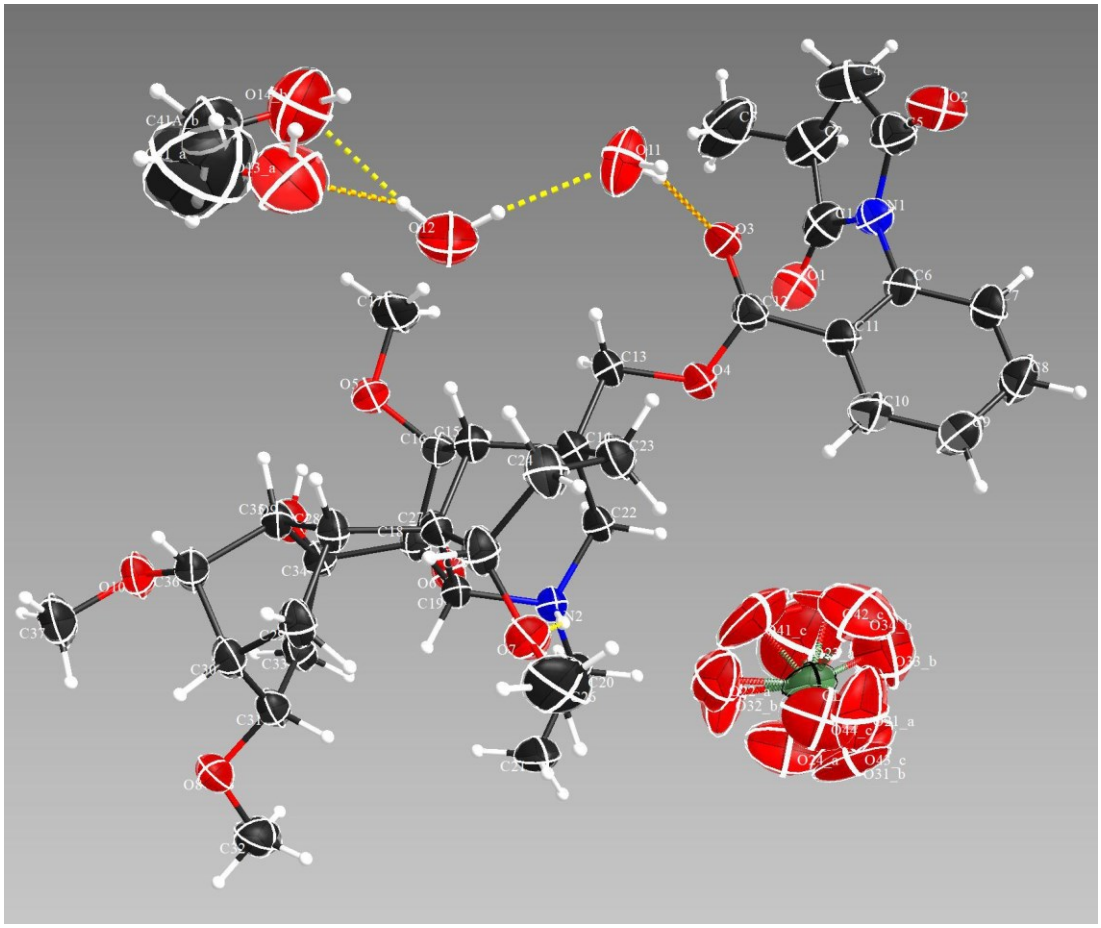

Table 112. Crystal data and structure refinement for s17phar14.

Identification code	s17phar14	
Empirical formula	C37.80 H57.80 Cl N2 O16.60	
Formula weight	841.31	
Temperature	199.99(16) K	
Wavelength	1.54184 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 10.9794(2) Å	α= 90°.
	b = 13.0176(2) Å	β= 90°.
	c = 28.5820(6) Å	γ = 90°.
Volume	4085.09(13) $Å^3$	
Z	4	
Density (calculated)	1.368 Mg/m^3	
Absorption coefficient	1.475 mm^{-1}	

F(000)	1794
Crystal size	0.250 x 0.200 x 0.050 mm^3
Theta range for data collection	3.092 to 73.155°.
Index ranges	-12<=h<=13, -10<=k<=16, -35<=l<=33
Reflections collected	28616
Independent reflections	8082 [R(int) = 0.0641]
Completeness to theta = 67.684°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.74008
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8082 / 107 / 651
Goodness-of-fit on F^2	1.038
Final R indices [I>2sigma(I)]	R1 = 0.0519, wR2 = 0.1333
R indices (all data)	R1 = 0.0641, wR2 = 0.1411
Absolute structure parameter	0.03(2)
Extinction coefficient	n/a
Largest diff. peak and hole	0.266 and -0.282 e.$Å^{-3}$

Table 113. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for s17phar14. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	8960(5)	599(4)	3960(2)	48(1)
C(2)	9327(6)	-202(4)	3607(2)	63(1)
C(3)	8334(10)	-389(7)	3254(3)	103(3)
C(4)	10501(7)	216(5)	3399(2)	74(2)
C(5)	10825(5)	1152(4)	3683(2)	49(1)
C(6)	9886(4)	2149(3)	4314(1)	34(1)
C(7)	10719(4)	2179(4)	4682(2)	45(1)
C(8)	10698(5)	2993(5)	4993(2)	54(1)
C(9)	9825(6)	3745(4)	4949(2)	57(1)
C(10)	8987(5)	3716(4)	4586(2)	46(1)
C(11)	9025(4)	2929(3)	4258(1)	34(1)
C(12)	8186(4)	2938(3)	3848(1)	34(1)
C(13)	6318(4)	3645(4)	3570(2)	42(1)
C(14)	5631(3)	4619(3)	3712(1)	35(1)

C(15)	4637(3)	4868(3)	3340(1)	33(1)
C(16)	3620(3)	4049(3)	3362(1)	33(1)
C(17)	3958(6)	3070(5)	2674(2)	67(2)
C(18)	2614(3)	4538(3)	3675(1)	30(1)
C(19)	3252(3)	5466(3)	3906(1)	28(1)
C(20)	3469(4)	4938(4)	4766(1)	44(1)
C(21)	2619(6)	5766(6)	4928(2)	68(2)
C(22)	5017(4)	4399(3)	4184(1)	36(1)
C(23)	6571(4)	5509(4)	3754(2)	43(1)
C(24)	6206(4)	6451(4)	3482(2)	45(1)
C(25)	4909(4)	6771(3)	3596(2)	38(1)
C(26)	5307(6)	8018(5)	4201(3)	79(2)
C(27)	3993(3)	5879(3)	3492(1)	31(1)
C(28)	3076(4)	6321(3)	3129(1)	33(1)
C(29)	2471(4)	7354(3)	3304(2)	38(1)
C(30)	1098(4)	7175(3)	3278(2)	37(1)
C(31)	590(3)	6680(3)	3720(2)	36(1)
C(32)	-992(4)	6951(4)	4267(2)	54(1)
C(33)	563(3)	5492(3)	3701(2)	36(1)
C(34)	1516(3)	4957(3)	3387(1)	32(1)
C(35)	1972(3)	5644(3)	2988(1)	33(1)
C(36)	1032(4)	6459(3)	2855(2)	38(1)
C(37)	-1009(5)	6755(4)	2628(2)	59(1)
N(1)	9911(3)	1307(3)	4002(1)	38(1)
N(2)	4092(3)	5197(3)	4308(1)	34(1)
O(1)	8023(4)	662(3)	4172(1)	59(1)
O(2)	11701(4)	1727(3)	3638(2)	63(1)
O(3)	8394(3)	2568(3)	3470(1)	44(1)
O(4)	7176(3)	3455(3)	3948(1)	46(1)
O(5)	3166(3)	3747(2)	2914(1)	42(1)
O(6)	2204(3)	3842(2)	4021(1)	39(1)
O(7)	4767(3)	7061(2)	4078(1)	46(1)
O(8)	-614(3)	7062(3)	3794(1)	46(1)
O(9)	881(3)	4077(2)	3207(1)	43(1)
O(10)	-119(3)	6011(2)	2752(1)	44(1)
O(11)	8633(4)	4058(4)	2662(2)	65(1)
O(12)	6374(6)	4825(7)	2384(2)	91(2)
O(13)	5982(11)	6119(13)	1598(5)	103(4)
C(41)	4970(30)	5840(40)	1288(15)	220(30)

O(14)	6110(20)	5022(19)	1401(8)	114(7)
C(41A)	5430(40)	5870(20)	1204(12)	94(9)
Cl	6824(1)	5964(1)	5316(1)	48(1)
O(21)	7610(19)	6767(18)	5396(9)	104(8)
O(22)	6116(12)	6489(9)	4919(4)	69(3)
O(23)	6590(30)	4986(16)	5285(10)	150(7)
O(24)	5802(15)	5832(14)	5610(7)	97(5)
O(31)	6880(20)	6567(15)	5689(6)	91(6)
O(32)	5669(18)	5900(20)	5136(10)	118(8)
O(33)	7550(20)	5120(20)	5535(11)	124(8)
O(34)	8042(18)	5970(20)	5094(8)	105(6)
O(41)	6580(30)	5550(20)	4913(7)	113(7)
O(42)	7430(18)	5186(12)	5130(7)	78(5)
O(43)	6610(30)	5834(19)	5802(6)	99(7)
O(44)	7170(20)	6960(13)	5283(9)	74(6)

Table 114. Bond lengths [Å] for s17phar14.

C(1)-O(1)	1.197(7)
C(1)-N(1)	1.397(7)
C(1)-C(2)	1.507(7)
C(2)-C(3)	1.506(10)
C(2)-C(4)	1.520(10)
C(2)-H(2)	1.0000
C(3)-H(3A)	0.9800
C(3)-H(3AB)	0.9800
C(3)-H(3AC)	0.9800
C(4)-C(5)	1.507(8)
C(4)-H(4A)	0.9900
C(4)-H(4AB)	0.9900
C(5)-O(2)	1.225(7)
C(5)-N(1)	1.371(6)
C(6)-C(7)	1.394(6)
C(6)-C(11)	1.397(6)
C(6)-N(1)	1.414(5)
C(7)-C(8)	1.383(7)

C(7)-H(7)	0.9500
C(8)-C(9)	1.376(8)
C(8)-H(8)	0.9500
C(9)-C(10)	1.388(7)
C(9)-H(9)	0.9500
C(10)-C(11)	1.388(6)
C(10)-H(10)	0.9500
C(11)-C(12)	1.490(5)
C(12)-O(3)	1.207(5)
C(12)-O(4)	1.328(5)
C(13)-O(4)	1.455(5)
C(13)-C(14)	1.530(6)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(22)	1.535(6)
C(14)-C(23)	1.556(6)
C(14)-C(15)	1.557(5)
C(15)-C(16)	1.546(5)
C(15)-C(27)	1.556(5)
C(15)-H(15)	1.0000
C(16)-O(5)	1.429(5)
C(16)-C(18)	1.558(5)
C(16)-H(16)	1.0000
C(17)-O(5)	1.416(6)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-O(6)	1.415(5)
C(18)-C(19)	1.544(5)
C(18)-C(34)	1.559(5)
C(19)-N(2)	1.515(4)
C(19)-C(27)	1.533(5)
C(19)-H(19)	1.0000
C(20)-C(21)	1.499(7)
C(20)-N(2)	1.515(5)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800

C(21)-H(21C)	0.9800
C(22)-N(2)	1.496(5)
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-C(24)	1.507(7)
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-C(25)	1.520(6)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-O(7)	1.438(6)
C(25)-C(27)	1.564(5)
C(25)-H(25)	1.0000
C(26)-O(7)	1.424(6)
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-C(28)	1.556(5)
C(28)-C(35)	1.552(5)
C(28)-C(29)	1.580(5)
C(28)-H(28)	1.0000
C(29)-C(30)	1.527(5)
C(29)-H(29A)	0.9900
C(29)-H(29B)	0.9900
C(30)-C(31)	1.524(6)
C(30)-C(36)	1.529(6)
C(30)-H(30)	1.0000
C(31)-O(8)	1.428(5)
C(31)-C(33)	1.547(5)
C(31)-H(31)	1.0000
C(32)-O(8)	1.421(7)
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-C(34)	1.546(5)
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(34)-O(9)	1.437(4)
C(34)-C(35)	1.531(6)

C(35)-C(36)	1.529(5)
C(35)-H(35)	1.0000
C(36)-O(10)	1.422(5)
C(36)-H(36)	1.0000
C(37)-O(10)	1.421(6)
C(37)-H(37A)	0.9800
C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800
N(2)-H(2A)	0.89(3)
O(6)-H(6)	0.87(3)
O(9)-H(9A)	0.87(3)
O(11)-H(11A)	0.88(3)
O(11)-H(11B)	0.88(3)
O(12)-H(12A)	0.86(3)
O(12)-H(12B)	0.86(3)
O(13)-C(41)	1.47(2)
O(13)-H(13)	0.8400
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
O(14)-C(41A)	1.44(2)
O(14)-H(14)	0.8400
C(41A)-H(41D)	0.9800
C(41A)-H(41E)	0.9800
C(41A)-H(41F)	0.9800
Cl-O(41)	1.301(16)
Cl-O(23)	1.303(19)
Cl-O(42)	1.323(11)
Cl-O(31)	1.326(12)
Cl-O(44)	1.353(16)
Cl-O(32)	1.371(16)
Cl-O(21)	1.375(19)
Cl-O(24)	1.412(12)
Cl-O(43)	1.420(15)
Cl-O(34)	1.481(17)
Cl-O(33)	1.49(3)
Cl-O(22)	1.536(10)
O(23)-O(24)	1.68(3)
O(33)-O(34)	1.76(4)

O(41)-O(42)	1.22(3)

Table 115. Bond angles [°] for s17phar14.

O(1)-C(1)-N(1)	123.6(5)
O(1)-C(1)-C(2)	128.1(5)
N(1)-C(1)-C(2)	108.3(5)
C(3)-C(2)-C(1)	111.6(6)
C(3)-C(2)-C(4)	114.2(6)
C(1)-C(2)-C(4)	103.9(5)
C(3)-C(2)-H(2)	109.0
C(1)-C(2)-H(2)	109.0
C(4)-C(2)-H(2)	109.0
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3AB)	109.5
H(3A)-C(3)-H(3AB)	109.5
C(2)-C(3)-H(3AC)	109.5
H(3A)-C(3)-H(3AC)	109.5
H(3AB)-C(3)-H(3AC)	109.5
C(5)-C(4)-C(2)	106.3(5)
C(5)-C(4)-H(4A)	110.5
C(2)-C(4)-H(4A)	110.5
C(5)-C(4)-H(4AB)	110.5
C(2)-C(4)-H(4AB)	110.5
H(4A)-C(4)-H(4AB)	108.7
O(2)-C(5)-N(1)	123.7(5)
O(2)-C(5)-C(4)	128.6(5)
N(1)-C(5)-C(4)	107.7(5)
C(7)-C(6)-C(11)	120.6(4)
C(7)-C(6)-N(1)	119.0(4)
C(11)-C(6)-N(1)	120.3(4)
C(8)-C(7)-C(6)	119.7(4)
C(8)-C(7)-H(7)	120.2
C(6)-C(7)-H(7)	120.2
C(9)-C(8)-C(7)	119.9(4)
C(9)-C(8)-H(8)	120.0
C(7)-C(8)-H(8)	120.0

C(8)-C(9)-C(10)	120.7(5)
C(8)-C(9)-H(9)	119.7
C(10)-C(9)-H(9)	119.7
C(9)-C(10)-C(11)	120.3(4)
C(9)-C(10)-H(10)	119.9
C(11)-C(10)-H(10)	119.9
C(10)-C(11)-C(6)	118.7(4)
C(10)-C(11)-C(12)	120.4(4)
C(6)-C(11)-C(12)	120.9(4)
O(3)-C(12)-O(4)	123.6(4)
O(3)-C(12)-C(11)	125.8(4)
O(4)-C(12)-C(11)	110.5(3)
O(4)-C(13)-C(14)	105.3(3)
O(4)-C(13)-H(13A)	110.7
C(14)-C(13)-H(13A)	110.7
O(4)-C(13)-H(13B)	110.7
C(14)-C(13)-H(13B)	110.7
H(13A)-C(13)-H(13B)	108.8
C(13)-C(14)-C(22)	107.1(3)
C(13)-C(14)-C(23)	108.0(3)
C(22)-C(14)-C(23)	111.3(4)
C(13)-C(14)-C(15)	109.7(3)
C(22)-C(14)-C(15)	109.3(3)
C(23)-C(14)-C(15)	111.3(3)
C(16)-C(15)-C(27)	104.1(3)
C(16)-C(15)-C(14)	109.6(3)
C(27)-C(15)-C(14)	107.7(3)
C(16)-C(15)-H(15)	111.7
C(27)-C(15)-H(15)	111.7
C(14)-C(15)-H(15)	111.7
O(5)-C(16)-C(15)	113.9(3)
O(5)-C(16)-C(18)	112.3(3)
C(15)-C(16)-C(18)	104.7(3)
O(5)-C(16)-H(16)	108.6
C(15)-C(16)-H(16)	108.6
C(18)-C(16)-H(16)	108.6
O(5)-C(17)-H(17A)	109.5
O(5)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5

O(5)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
O(6)-C(18)-C(19)	110.2(3)
O(6)-C(18)-C(16)	111.5(3)
C(19)-C(18)-C(16)	104.1(3)
O(6)-C(18)-C(34)	110.4(3)
C(19)-C(18)-C(34)	107.6(3)
C(16)-C(18)-C(34)	112.8(3)
N(2)-C(19)-C(27)	110.1(3)
N(2)-C(19)-C(18)	114.8(3)
C(27)-C(19)-C(18)	100.7(3)
N(2)-C(19)-H(19)	110.3
C(27)-C(19)-H(19)	110.3
C(18)-C(19)-H(19)	110.3
C(21)-C(20)-N(2)	112.8(4)
C(21)-C(20)-H(20A)	109.0
N(2)-C(20)-H(20A)	109.0
C(21)-C(20)-H(20B)	109.0
N(2)-C(20)-H(20B)	109.0
H(20A)-C(20)-H(20B)	107.8
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
N(2)-C(22)-C(14)	112.2(3)
N(2)-C(22)-H(22A)	109.2
C(14)-C(22)-H(22A)	109.2
N(2)-C(22)-H(22B)	109.2
C(14)-C(22)-H(22B)	109.2
H(22A)-C(22)-H(22B)	107.9
C(24)-C(23)-C(14)	112.9(3)
C(24)-C(23)-H(23A)	109.0
C(14)-C(23)-H(23A)	109.0
C(24)-C(23)-H(23B)	109.0
C(14)-C(23)-H(23B)	109.0
H(23A)-C(23)-H(23B)	107.8

C(23)-C(24)-C(25)	111.2(4)
C(23)-C(24)-H(24A)	109.4
C(25)-C(24)-H(24A)	109.4
C(23)-C(24)-H(24B)	109.4
C(25)-C(24)-H(24B)	109.4
H(24A)-C(24)-H(24B)	108.0
O(7)-C(25)-C(24)	112.3(4)
O(7)-C(25)-C(27)	107.9(3)
C(24)-C(25)-C(27)	111.0(3)
O(7)-C(25)-H(25)	108.5
C(24)-C(25)-H(25)	108.5
C(27)-C(25)-H(25)	108.5
O(7)-C(26)-H(26A)	109.5
O(7)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
O(7)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(19)-C(27)-C(28)	107.5(3)
C(19)-C(27)-C(15)	99.2(3)
C(28)-C(27)-C(15)	114.9(3)
C(19)-C(27)-C(25)	117.1(3)
C(28)-C(27)-C(25)	105.5(3)
C(15)-C(27)-C(25)	112.9(3)
C(35)-C(28)-C(27)	117.9(3)
C(35)-C(28)-C(29)	103.7(3)
C(27)-C(28)-C(29)	112.1(3)
C(35)-C(28)-H(28)	107.5
C(27)-C(28)-H(28)	107.5
C(29)-C(28)-H(28)	107.5
C(30)-C(29)-C(28)	105.6(3)
C(30)-C(29)-H(29A)	110.6
C(28)-C(29)-H(29A)	110.6
C(30)-C(29)-H(29B)	110.6
C(28)-C(29)-H(29B)	110.6
H(29A)-C(29)-H(29B)	108.7
C(31)-C(30)-C(29)	112.7(3)
C(31)-C(30)-C(36)	112.4(3)
C(29)-C(30)-C(36)	100.3(3)

C(31)-C(30)-H(30)	110.4
C(29)-C(30)-H(30)	110.4
C(36)-C(30)-H(30)	110.4
O(8)-C(31)-C(30)	108.4(3)
O(8)-C(31)-C(33)	109.6(3)
C(30)-C(31)-C(33)	113.7(4)
O(8)-C(31)-H(31)	108.4
C(30)-C(31)-H(31)	108.4
C(33)-C(31)-H(31)	108.4
O(8)-C(32)-H(32A)	109.5
O(8)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
O(8)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(34)-C(33)-C(31)	117.2(3)
C(34)-C(33)-H(33A)	108.0
C(31)-C(33)-H(33A)	108.0
C(34)-C(33)-H(33B)	108.0
C(31)-C(33)-H(33B)	108.0
H(33A)-C(33)-H(33B)	107.2
O(9)-C(34)-C(35)	110.9(3)
O(9)-C(34)-C(33)	103.8(3)
C(35)-C(34)-C(33)	113.0(3)
O(9)-C(34)-C(18)	106.6(3)
C(35)-C(34)-C(18)	110.2(3)
C(33)-C(34)-C(18)	111.9(3)
C(36)-C(35)-C(34)	111.7(3)
C(36)-C(35)-C(28)	101.4(3)
C(34)-C(35)-C(28)	113.2(3)
C(36)-C(35)-H(35)	110.1
C(34)-C(35)-H(35)	110.1
C(28)-C(35)-H(35)	110.1
O(10)-C(36)-C(30)	117.1(4)
O(10)-C(36)-C(35)	111.5(3)
C(30)-C(36)-C(35)	101.2(3)
O(10)-C(36)-H(36)	108.9
C(30)-C(36)-H(36)	108.9
C(35)-C(36)-H(36)	108.9

O(10)-C(37)-H(37A)	109.5
O(10)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
O(10)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
C(5)-N(1)-C(1)	113.2(4)
C(5)-N(1)-C(6)	123.2(4)
C(1)-N(1)-C(6)	123.4(4)
C(22)-N(2)-C(19)	113.1(3)
C(22)-N(2)-C(20)	110.9(3)
C(19)-N(2)-C(20)	115.6(3)
C(22)-N(2)-H(2A)	110(5)
C(19)-N(2)-H(2A)	96(5)
C(20)-N(2)-H(2A)	110(5)
C(12)-O(4)-C(13)	117.9(3)
C(17)-O(5)-C(16)	113.0(3)
C(18)-O(6)-H(6)	93(10)
C(26)-O(7)-C(25)	114.8(5)
C(32)-O(8)-C(31)	112.2(4)
C(34)-O(9)-H(9A)	109(5)
C(37)-O(10)-C(36)	112.5(4)
H(11A)-O(11)-H(11B)	101(4)
H(12A)-O(12)-H(12B)	105(4)
C(41)-O(13)-H(13)	109.5
O(13)-C(41)-H(41A)	109.5
O(13)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
O(13)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(41A)-O(14)-H(14)	109.5
O(14)-C(41A)-H(41D)	109.5
O(14)-C(41A)-H(41E)	109.5
H(41D)-C(41A)-H(41E)	109.5
O(14)-C(41A)-H(41F)	109.5
H(41D)-C(41A)-H(41F)	109.5
H(41E)-C(41A)-H(41F)	109.5
O(41)-Cl-O(42)	55.2(15)

O(41)-Cl-O(44)	113.4(17)
O(42)-Cl-O(44)	124.5(13)
O(31)-Cl-O(32)	112.4(16)
O(23)-Cl-O(21)	151.5(16)
O(23)-Cl-O(24)	76.3(15)
O(21)-Cl-O(24)	119.5(14)
O(41)-Cl-O(43)	141.4(15)
O(42)-Cl-O(43)	112.7(14)
O(44)-Cl-O(43)	103.2(14)
O(31)-Cl-O(34)	107.3(15)
O(32)-Cl-O(34)	132.4(15)
O(31)-Cl-O(33)	94.0(15)
O(32)-Cl-O(33)	127.5(17)
O(34)-Cl-O(33)	72.8(15)
O(23)-Cl-O(22)	106.6(13)
O(21)-Cl-O(22)	95.9(10)
O(24)-Cl-O(22)	95.3(10)
Cl-O(23)-O(24)	54.8(11)
Cl-O(24)-O(23)	48.9(9)
Cl-O(33)-O(34)	53.4(12)
Cl-O(34)-O(33)	53.9(11)
O(42)-O(41)-Cl	63.3(12)
O(41)-O(42)-Cl	61.5(11)

Table 116. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for s17phar14. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	62(3)	38(2)	43(2)	8(2)	-5(2)	2(2)
C(2)	93(4)	36(2)	59(3)	-2(2)	0(3)	-1(3)
C(3)	140(8)	96(6)	74(5)	-30(4)	-20(5)	-4(6)
C(4)	103(5)	52(3)	68(4)	-17(3)	22(4)	12(3)
C(5)	56(3)	46(2)	46(2)	4(2)	4(2)	13(2)
C(6)	37(2)	35(2)	30(2)	4(2)	-1(2)	4(2)
C(7)	44(2)	52(2)	38(2)	10(2)	-5(2)	10(2)

C(8)	56(3)	68(3)	37(2)	-1(2)	-15(2)	-2(3)
C(9)	70(3)	60(3)	41(2)	-13(2)	-6(2)	1(3)
C(10)	52(2)	43(2)	44(2)	-8(2)	-5(2)	11(2)
C(11)	36(2)	36(2)	31(2)	2(2)	0(2)	6(2)
C(12)	34(2)	32(2)	36(2)	3(2)	0(2)	8(2)
C(13)	35(2)	53(2)	37(2)	-4(2)	-7(2)	20(2)
C(14)	30(2)	42(2)	34(2)	-2(2)	-3(2)	9(2)
C(15)	31(2)	36(2)	33(2)	-2(2)	-3(2)	3(2)
C(16)	34(2)	31(2)	34(2)	-5(2)	-5(1)	6(2)
C(17)	63(3)	68(3)	69(4)	-43(3)	-14(3)	23(3)
C(18)	31(2)	24(2)	35(2)	2(1)	-3(1)	2(1)
C(19)	29(2)	29(2)	26(2)	-2(1)	-4(1)	6(1)
C(20)	47(2)	60(3)	26(2)	1(2)	0(2)	19(2)
C(21)	72(3)	95(5)	36(2)	-11(3)	4(2)	39(3)
C(22)	34(2)	40(2)	34(2)	2(2)	-3(2)	13(2)
C(23)	29(2)	50(2)	51(2)	0(2)	-4(2)	3(2)
C(24)	32(2)	49(2)	53(3)	3(2)	-1(2)	-7(2)
C(25)	33(2)	34(2)	48(2)	1(2)	-9(2)	-2(2)
C(26)	64(3)	55(3)	117(6)	-44(4)	-9(4)	-15(3)
C(27)	28(2)	32(2)	33(2)	1(2)	-4(1)	5(2)
C(28)	33(2)	33(2)	34(2)	5(1)	-7(2)	4(2)
C(29)	38(2)	28(2)	48(2)	4(2)	-9(2)	1(2)
C(30)	35(2)	30(2)	47(2)	-2(2)	-11(2)	8(2)
C(31)	29(2)	33(2)	46(2)	-6(2)	-9(2)	4(2)
C(32)	39(2)	60(3)	62(3)	-17(2)	3(2)	3(2)
C(33)	29(2)	34(2)	44(2)	-1(2)	-4(2)	0(2)
C(34)	31(2)	26(2)	38(2)	-6(1)	-8(2)	0(1)
C(35)	32(2)	35(2)	31(2)	-1(1)	-8(1)	6(2)
C(36)	38(2)	36(2)	40(2)	1(2)	-13(2)	5(2)
C(37)	49(2)	58(3)	70(3)	-4(3)	-26(3)	16(2)
N(1)	47(2)	32(2)	34(2)	2(1)	-1(1)	11(1)
N(2)	34(2)	38(2)	30(2)	-3(1)	-6(1)	10(1)
O(1)	61(2)	64(2)	52(2)	5(2)	0(2)	-16(2)
O(2)	58(2)	65(2)	67(2)	-6(2)	19(2)	3(2)
O(3)	46(2)	50(2)	35(2)	-5(1)	-3(1)	19(1)
O(4)	40(2)	62(2)	35(2)	-1(1)	-3(1)	24(2)
O(5)	44(1)	42(2)	42(2)	-16(1)	-10(1)	8(1)
O(6)	40(1)	32(1)	45(2)	9(1)	-2(1)	2(1)
O(7)	42(2)	38(2)	57(2)	-15(1)	-8(1)	-3(1)

O(8)	35(1)	50(2)	53(2)	-10(1)	-5(1)	13(1)
O(9)	37(1)	33(1)	59(2)	-10(1)	-14(1)	-4(1)
O(10)	37(1)	45(2)	51(2)	-4(1)	-17(1)	7(1)
O(11)	64(2)	73(2)	58(2)	10(2)	-22(2)	-20(2)
O(12)	66(3)	144(7)	62(4)	6(4)	15(3)	19(4)
O(13)	74(6)	137(10)	98(8)	-1(8)	11(6)	-27(7)
C(41)	250(30)	210(30)	200(30)	-40(20)	-10(20)	0(20)
O(14)	108(13)	145(17)	89(12)	-19(13)	-21(11)	3(14)
C(41A)	109(17)	92(16)	81(15)	-44(13)	-38(14)	18(14)
Cl	54(1)	40(1)	49(1)	-12(1)	7(1)	-13(1)
O(21)	90(11)	103(15)	119(14)	-19(11)	-43(10)	-41(10)
O(22)	80(7)	68(6)	58(6)	11(5)	-15(5)	6(6)
O(23)	187(13)	90(9)	172(13)	-9(10)	-21(12)	-36(10)
O(24)	85(8)	107(9)	98(9)	5(8)	51(7)	-7(7)
O(31)	135(14)	72(10)	65(9)	-51(9)	8(10)	0(10)
O(32)	68(10)	158(18)	129(16)	-29(15)	-56(11)	-22(12)
O(33)	109(11)	118(12)	146(14)	1(11)	-32(11)	13(10)
O(34)	78(9)	136(12)	99(10)	-2(10)	38(8)	-4(10)
O(41)	147(13)	128(12)	65(8)	-51(9)	-21(9)	-30(10)
O(42)	95(9)	59(7)	82(9)	-17(6)	50(8)	37(7)
O(43)	152(17)	107(13)	38(7)	-7(8)	36(10)	-45(13)
O(44)	84(13)	29(6)	107(15)	9(8)	23(11)	-25(8)

Table 117. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for s17phar14.

	x	y	z	U(eq)
H(2)	9507	-860	3774	75
H(3A)	8620	-881	3019	155
H(3AB)	8122	260	3100	155
H(3AC)	7614	-667	3412	155
H(4A)	11157	-304	3419	89
H(4AB)	10380	402	3067	89
H(7)	11297	1643	4719	54
H(8)	11286	3033	5236	64

H(9)	9796	4290	5170	69
H(10)	8384	4237	4561	56
H(13A)	5749	3061	3534	50
H(13B)	6754	3750	3270	50
H(15)	4992	4925	3019	40
H(16)	3946	3426	3524	39
H(17A)	3612	2903	2367	100
H(17B)	4057	2438	2857	100
H(17C)	4753	3399	2632	100
H(19)	2636	5985	4008	34
H(20A)	3006	4290	4728	53
H(20B)	4097	4822	5009	53
H(21A)	2354	5619	5249	101
H(21B)	1907	5789	4721	101
H(21C)	3039	6429	4920	101
H(22A)	4615	3718	4170	43
H(22B)	5646	4371	4431	43
H(23A)	6665	5695	4088	52
H(23B)	7372	5266	3639	52
H(24A)	6274	6308	3143	54
H(24B)	6769	7022	3558	54
H(25)	4689	7373	3396	46
H(26A)	5046	8216	4516	118
H(26B)	5053	8545	3976	118
H(26C)	6196	7951	4194	118
H(28)	3542	6481	2837	40
H(29A)	2723	7509	3629	46
H(29B)	2712	7935	3100	46
H(30)	665	7834	3211	44
H(31)	1109	6893	3990	43
H(32A)	-1761	7319	4314	80
H(32B)	-368	7237	4475	80
H(32C)	-1108	6221	4338	80
H(33A)	668	5231	4024	43
H(33B)	-256	5278	3594	43
H(35)	2182	5215	2709	39
H(36)	1328	6837	2572	45
H(37A)	-1739	6407	2511	89
H(37B)	-681	7206	2384	89

H(37C)	-1221	7165	2904	89
H(2A)	4450(60)	5810(30)	4330(20)	70(20)
H(6)	2290(180)	3310(100)	3840(60)	290(100)
H(9A)	1380(50)	3710(50)	3040(20)	70(20)
H(11A)	9180(40)	4510(40)	2760(20)	58(17)
H(11B)	8690(90)	3580(60)	2880(30)	150(50)
H(12A)	6320(70)	5000(80)	2094(15)	90(30)
H(12B)	7150(30)	4760(70)	2430(30)	70(30)
H(13)	6589	6286	1436	155
H(41A)	4793	6417	1076	330
H(41B)	4242	5694	1477	330
H(41C)	5186	5235	1105	330
H(14)	6798	5233	1489	171
H(41D)	5964	6462	1168	141
H(41E)	4753	6041	1413	141
H(41F)	5108	5665	898	141

Table 118. Torsion angles [°] for s17phar14.

O(1)-C(1)-C(2)-C(3)	47.1(8)
N(1)-C(1)-C(2)-C(3)	-131.8(6)
O(1)-C(1)-C(2)-C(4)	170.6(5)
N(1)-C(1)-C(2)-C(4)	-8.3(6)
C(3)-C(2)-C(4)-C(5)	128.7(6)
C(1)-C(2)-C(4)-C(5)	6.9(7)
C(2)-C(4)-C(5)-O(2)	179.9(5)
C(2)-C(4)-C(5)-N(1)	-3.3(6)
C(11)-C(6)-C(7)-C(8)	-0.6(7)
N(1)-C(6)-C(7)-C(8)	-179.4(4)
C(6)-C(7)-C(8)-C(9)	2.8(8)
C(7)-C(8)-C(9)-C(10)	-2.2(9)
C(8)-C(9)-C(10)-C(11)	-0.5(9)
C(9)-C(10)-C(11)-C(6)	2.7(7)
C(9)-C(10)-C(11)-C(12)	-175.4(5)
C(7)-C(6)-C(11)-C(10)	-2.2(6)
N(1)-C(6)-C(11)-C(10)	176.6(4)

C(7)-C(6)-C(11)-C(12)	176.0(4)
N(1)-C(6)-C(11)-C(12)	-5.2(6)
C(10)-C(11)-C(12)-O(3)	150.6(5)
C(6)-C(11)-C(12)-O(3)	-27.5(7)
C(10)-C(11)-C(12)-O(4)	-26.8(6)
C(6)-C(11)-C(12)-O(4)	155.1(4)
O(4)-C(13)-C(14)-C(22)	-58.8(4)
O(4)-C(13)-C(14)-C(23)	61.2(4)
O(4)-C(13)-C(14)-C(15)	-177.3(3)
C(13)-C(14)-C(15)-C(16)	69.0(4)
C(22)-C(14)-C(15)-C(16)	-48.2(4)
C(23)-C(14)-C(15)-C(16)	-171.5(3)
C(13)-C(14)-C(15)-C(27)	-178.3(3)
C(22)-C(14)-C(15)-C(27)	64.5(4)
C(23)-C(14)-C(15)-C(27)	-58.8(4)
C(27)-C(15)-C(16)-O(5)	104.7(3)
C(14)-C(15)-C(16)-O(5)	-140.3(3)
C(27)-C(15)-C(16)-C(18)	-18.4(4)
C(14)-C(15)-C(16)-C(18)	96.6(3)
O(5)-C(16)-C(18)-O(6)	103.5(4)
C(15)-C(16)-C(18)-O(6)	-132.4(3)
O(5)-C(16)-C(18)-C(19)	-137.7(3)
C(15)-C(16)-C(18)-C(19)	-13.6(4)
O(5)-C(16)-C(18)-C(34)	-21.3(4)
C(15)-C(16)-C(18)-C(34)	102.8(3)
O(6)-C(18)-C(19)-N(2)	42.3(4)
C(16)-C(18)-C(19)-N(2)	-77.4(4)
C(34)-C(18)-C(19)-N(2)	162.6(3)
O(6)-C(18)-C(19)-C(27)	160.5(3)
C(16)-C(18)-C(19)-C(27)	40.8(3)
C(34)-C(18)-C(19)-C(27)	-79.1(3)
C(13)-C(14)-C(22)-N(2)	-167.0(3)
C(23)-C(14)-C(22)-N(2)	75.1(4)
C(15)-C(14)-C(22)-N(2)	-48.2(5)
C(13)-C(14)-C(23)-C(24)	128.7(4)
C(22)-C(14)-C(23)-C(24)	-113.9(4)
C(15)-C(14)-C(23)-C(24)	8.3(5)
C(14)-C(23)-C(24)-C(25)	50.8(5)
C(23)-C(24)-C(25)-O(7)	63.1(5)

C(23)-C(24)-C(25)-C(27)	-57.7(5)
N(2)-C(19)-C(27)-C(28)	-170.0(3)
C(18)-C(19)-C(27)-C(28)	68.4(3)
N(2)-C(19)-C(27)-C(15)	70.2(3)
C(18)-C(19)-C(27)-C(15)	-51.5(3)
N(2)-C(19)-C(27)-C(25)	-51.5(4)
C(18)-C(19)-C(27)-C(25)	-173.1(3)
C(16)-C(15)-C(27)-C(19)	43.4(3)
C(14)-C(15)-C(27)-C(19)	-72.9(3)
C(16)-C(15)-C(27)-C(28)	-70.9(4)
C(14)-C(15)-C(27)-C(28)	172.8(3)
C(16)-C(15)-C(27)-C(25)	168.0(3)
C(14)-C(15)-C(27)-C(25)	51.8(4)
O(7)-C(25)-C(27)-C(19)	-4.4(4)
C(24)-C(25)-C(27)-C(19)	119.1(4)
O(7)-C(25)-C(27)-C(28)	115.2(3)
C(24)-C(25)-C(27)-C(28)	-121.4(4)
O(7)-C(25)-C(27)-C(15)	-118.6(3)
C(24)-C(25)-C(27)-C(15)	4.8(5)
C(19)-C(27)-C(28)-C(35)	-48.9(4)
C(15)-C(27)-C(28)-C(35)	60.5(5)
C(25)-C(27)-C(28)-C(35)	-174.5(3)
C(19)-C(27)-C(28)-C(29)	71.5(4)
C(15)-C(27)-C(28)-C(29)	-179.2(3)
C(25)-C(27)-C(28)-C(29)	-54.2(4)
C(35)-C(28)-C(29)-C(30)	3.2(4)
C(27)-C(28)-C(29)-C(30)	-125.1(4)
C(28)-C(29)-C(30)-C(31)	86.9(4)
C(28)-C(29)-C(30)-C(36)	-32.8(4)
C(29)-C(30)-C(31)-O(8)	146.7(3)
C(36)-C(30)-C(31)-O(8)	-100.9(4)
C(29)-C(30)-C(31)-C(33)	-91.2(4)
C(36)-C(30)-C(31)-C(33)	21.2(4)
O(8)-C(31)-C(33)-C(34)	148.9(3)
C(30)-C(31)-C(33)-C(34)	27.4(5)
C(31)-C(33)-C(34)-O(9)	-145.2(3)
C(31)-C(33)-C(34)-C(35)	-24.9(5)
C(31)-C(33)-C(34)-C(18)	100.2(4)
O(6)-C(18)-C(34)-O(9)	-55.2(4)

C(19)-C(18)-C(34)-O(9)	-175.5(3)
C(16)-C(18)-C(34)-O(9)	70.2(4)
O(6)-C(18)-C(34)-C(35)	-175.6(3)
C(19)-C(18)-C(34)-C(35)	64.1(4)
C(16)-C(18)-C(34)-C(35)	-50.2(4)
O(6)-C(18)-C(34)-C(33)	57.7(4)
C(19)-C(18)-C(34)-C(33)	-62.6(4)
C(16)-C(18)-C(34)-C(33)	-176.9(3)
O(9)-C(34)-C(35)-C(36)	90.3(4)
C(33)-C(34)-C(35)-C(36)	-25.9(4)
C(18)-C(34)-C(35)-C(36)	-151.9(3)
O(9)-C(34)-C(35)-C(28)	-156.0(3)
C(33)-C(34)-C(35)-C(28)	87.8(4)
C(18)-C(34)-C(35)-C(28)	-38.3(4)
C(27)-C(28)-C(35)-C(36)	152.4(3)
C(29)-C(28)-C(35)-C(36)	27.8(4)
C(27)-C(28)-C(35)-C(34)	32.6(5)
C(29)-C(28)-C(35)-C(34)	-92.0(4)
C(31)-C(30)-C(36)-O(10)	52.5(4)
C(29)-C(30)-C(36)-O(10)	172.4(3)
C(31)-C(30)-C(36)-C(35)	-68.9(4)
C(29)-C(30)-C(36)-C(35)	51.1(4)
C(34)-C(35)-C(36)-O(10)	-53.7(4)
C(28)-C(35)-C(36)-O(10)	-174.5(3)
C(34)-C(35)-C(36)-C(30)	71.5(4)
C(28)-C(35)-C(36)-C(30)	-49.3(4)
O(2)-C(5)-N(1)-C(1)	174.9(5)
C(4)-C(5)-N(1)-C(1)	-2.1(6)
O(2)-C(5)-N(1)-C(6)	-0.1(7)
C(4)-C(5)-N(1)-C(6)	-177.1(4)
O(1)-C(1)-N(1)-C(5)	-172.1(5)
C(2)-C(1)-N(1)-C(5)	6.8(5)
O(1)-C(1)-N(1)-C(6)	2.8(7)
C(2)-C(1)-N(1)-C(6)	-178.2(4)
C(7)-C(6)-N(1)-C(5)	-70.9(5)
C(11)-C(6)-N(1)-C(5)	110.3(5)
C(7)-C(6)-N(1)-C(1)	114.7(5)
C(11)-C(6)-N(1)-C(1)	-64.2(5)
C(14)-C(22)-N(2)-C(19)	46.1(5)

C(14)-C(22)-N(2)-C(20)	177.9(3)
C(27)-C(19)-N(2)-C(22)	-59.8(4)
C(18)-C(19)-N(2)-C(22)	53.0(5)
C(27)-C(19)-N(2)-C(20)	170.8(3)
C(18)-C(19)-N(2)-C(20)	-76.4(4)
C(21)-C(20)-N(2)-C(22)	174.6(4)
C(21)-C(20)-N(2)-C(19)	-54.9(5)
O(3)-C(12)-O(4)-C(13)	-4.6(6)
C(11)-C(12)-O(4)-C(13)	172.8(4)
C(14)-C(13)-O(4)-C(12)	-153.8(4)
C(15)-C(16)-O(5)-C(17)	76.8(5)
C(18)-C(16)-O(5)-C(17)	-164.4(4)
C(24)-C(25)-O(7)-C(26)	72.1(5)
C(27)-C(25)-O(7)-C(26)	-165.2(4)
C(30)-C(31)-O(8)-C(32)	-158.7(4)
C(33)-C(31)-O(8)-C(32)	76.7(5)
C(30)-C(36)-O(10)-C(37)	64.1(5)
C(35)-C(36)-O(10)-C(37)	179.9(4)
O(21)-Cl-O(23)-O(24)	128(3)
O(22)-Cl-O(23)-O(24)	-91.5(11)
O(21)-Cl-O(24)-O(23)	-154.3(16)
O(22)-Cl-O(24)-O(23)	105.8(14)
O(31)-Cl-O(33)-O(34)	-106.9(16)
O(32)-Cl-O(33)-O(34)	131(2)
O(31)-Cl-O(34)-O(33)	88.8(16)
O(32)-Cl-O(34)-O(33)	-126(2)
O(44)-Cl-O(41)-O(42)	116.8(17)
O(43)-Cl-O(41)-O(42)	-83(3)
O(44)-Cl-O(42)-O(41)	-96(2)
O(43)-Cl-O(42)-O(41)	137.8(19)

Table 119. Hydrogen bonds for s17phar14 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2A)...O(7)	0.89(3)	1.81(4)	2.620(5)	150(6)
N(2)-H(2A)...O(22)	0.89(3)	2.64(6)	3.288(13)	130(6)

O(6)-H(6)...O(2)#1	0.87(3)	2.24(11)	3.015(5)	149(18)
O(9)-H(9A)...O(5)	0.87(3)	2.00(5)	2.679(5)	135(6)
O(11)-H(11A)...O(9)#2	0.88(3)	2.33(5)	2.917(5)	124(5)
O(11)-H(11A)...O(10)#2	0.88(3)	2.10(4)	2.899(5)	149(5)
O(11)-H(11B)...O(3)	0.88(3)	2.17(4)	3.026(5)	165(11)
O(12)-H(12A)...O(13)	0.86(3)	2.07(6)	2.840(17)	149(10)
O(12)-H(12A)...O(14)	0.86(3)	1.99(5)	2.83(2)	166(11)
O(12)-H(12B)...O(11)	0.86(3)	1.98(4)	2.790(8)	155(8)
O(13)-H(13)...O(2)#3	0.84	1.97	2.749(12)	152.7
O(14)-H(14)...O(2)#3	0.84	2.58	3.27(3)	141.2

Symmetry transformations used to generate equivalent atoms:

#1 x-1,y,z #2 x+1,y,z #3 -x+2,y+1/2,-z+1/2

s18phar1: methyllycaconitine perchlorate monoacetonitrile dichloroform solvate (**31c**)

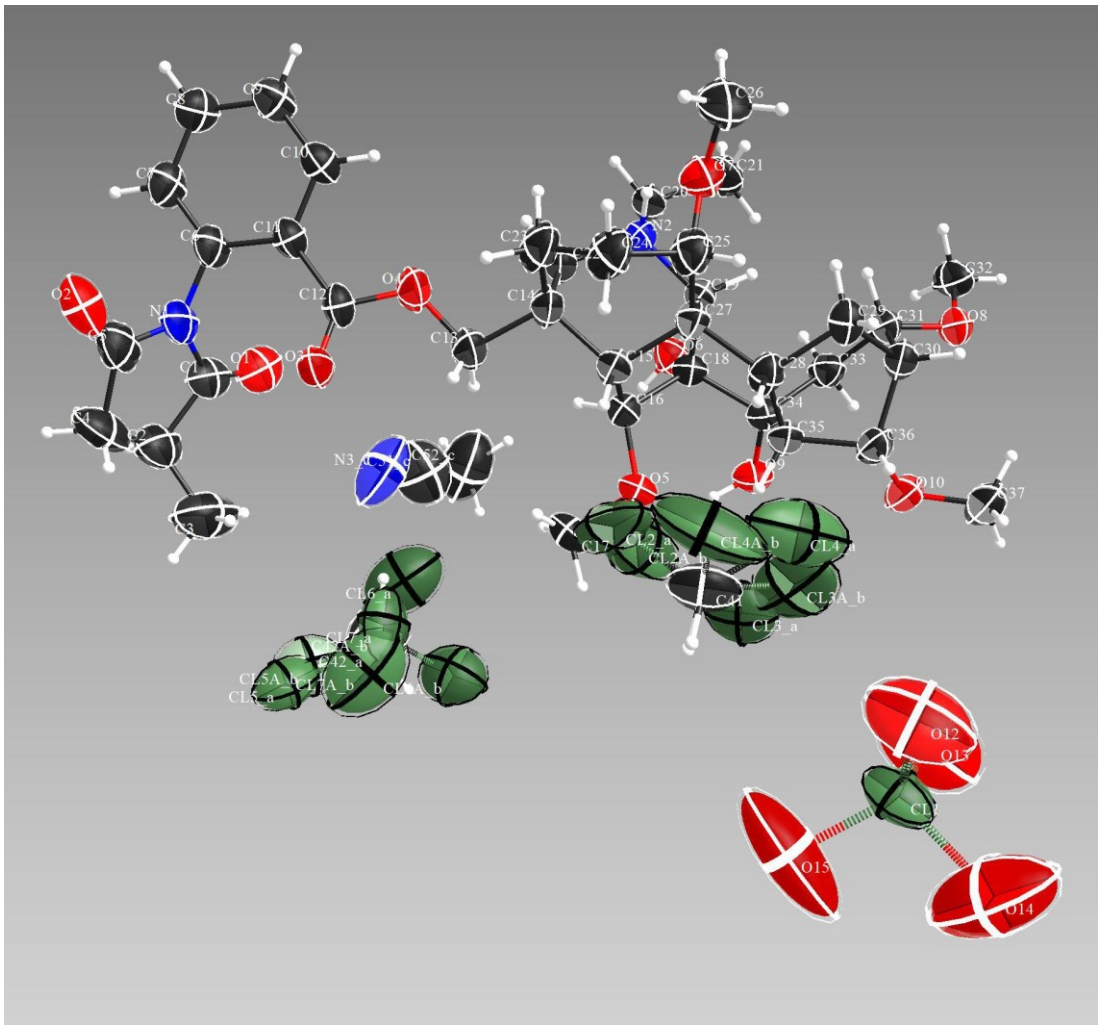

Table 120. Crystal data and structure refinement for s18phar1.

Identification code	s18phar1	
Empirical formula	C79 H108 Cl11 N5 O28	
Formula weight	1965.65	
Temperature	150.01(10) K	
Wavelength	1.54184 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 12.9258(11) Å	α= 90°.
	b = 10.9422(6) Å	β= 107.590(11)°.
	c = 17.6294(15) Å	γ = 90°.
Volume	2376.9(3) $Å^3$	
Z	1	
Density (calculated)	1.373 Mg/m^3	
Absorption coefficient	3.584 mm^{-1}	
F(000)	1028	
Crystal size	0.353 x 0.101 x 0.036 mm^3	
Theta range for data collection	3.587 to 68.528°.	
Index ranges	-14<=h<=15, -10<=k<=13, -21<=l<=19	
Reflections collected	17037	
Independent reflections	7045 [R(int) = 0.0474]	
Completeness to theta = 67.684°	99.9 %	
Absorption correction	Gaussian	
Max. and min. transmission	1.000 and 0.568	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7045 / 85 / 653	
Goodness-of-fit on F^2	1.029	
Final R indices [I>2sigma(I)]	R1 = 0.0669, wR2 = 0.1803	
R indices (all data)	R1 = 0.0766, wR2 = 0.1949	
Absolute structure parameter	-0.001(16)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.548 and -0.389 $e.Å^{-3}$	

Table 121. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for s18phar1. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	3061(4)	219(6)	8210(3)	52(1)
N(2)	7260(4)	6093(4)	8893(2)	41(1)
O(1)	2436(4)	2125(6)	8423(4)	72(1)
O(2)	3303(5)	-1628(7)	7692(4)	81(2)
O(3)	4006(3)	1845(4)	7409(2)	54(1)
O(4)	5264(4)	3002(5)	8249(3)	63(1)
O(5)	4735(4)	7118(5)	6604(3)	58(1)
O(6)	5697(3)	8004(4)	8497(2)	48(1)
O(7)	8945(4)	5470(4)	8436(3)	57(1)
O(8)	8700(3)	10920(4)	8054(2)	50(1)
O(9)	5276(3)	9396(5)	7136(3)	56(1)
O(10)	6838(4)	10479(4)	6320(3)	59(1)
C(1)	2286(5)	1187(8)	8078(4)	58(2)
C(2)	1275(6)	767(9)	7436(5)	74(2)
C(3)	889(10)	1736(16)	6816(7)	119(5)
C(4)	1605(6)	-447(12)	7174(5)	89(3)
C(5)	2739(6)	-729(9)	7702(5)	66(2)
C(6)	4095(4)	272(6)	8806(3)	47(1)
C(7)	4319(5)	-535(7)	9422(4)	52(1)
C(8)	5314(5)	-497(7)	10020(4)	55(2)
C(9)	6052(5)	404(7)	9992(4)	56(1)
C(10)	5822(4)	1233(6)	9366(3)	48(1)
C(11)	4841(4)	1178(5)	8754(3)	42(1)
C(12)	4631(4)	2015(5)	8062(3)	42(1)
C(13)	5175(6)	3882(7)	7623(4)	58(2)
C(14)	6249(5)	4592(5)	7855(3)	48(1)
C(15)	6200(5)	5642(5)	7250(3)	45(1)
C(16)	5402(4)	6627(6)	7344(3)	46(1)
C(17)	3784(6)	6398(9)	6255(5)	79(2)
C(18)	6124(4)	7629(5)	7879(3)	41(1)
C(19)	7218(4)	6979(5)	8220(3)	38(1)
C(20)	7320(5)	6663(6)	9692(3)	49(1)
C(21)	8168(5)	7646(7)	9951(4)	59(2)
C(22)	6380(5)	5151(6)	8681(3)	49(1)

C(23)	7170(6)	3662(6)	7867(4)	60(2)
C(24)	7900(7)	4095(6)	7399(4)	61(2)
C(25)	8300(5)	5389(6)	7620(4)	54(1)
C(26)	10008(6)	4958(9)	8622(7)	83(3)
C(27)	7326(4)	6287(5)	7494(3)	42(1)
C(28)	7458(5)	7260(5)	6886(3)	44(1)
C(29)	8619(5)	7865(5)	7158(3)	46(1)
C(30)	8411(5)	9252(5)	7141(3)	44(1)
C(31)	8266(5)	9697(5)	7927(3)	41(1)
C(32)	8945(5)	11279(6)	8856(4)	54(1)
C(33)	7077(5)	9709(5)	7932(3)	44(1)
C(34)	6290(4)	8774(5)	7403(3)	42(1)
C(35)	6663(4)	8355(6)	6687(3)	45(1)
C(36)	7360(5)	9336(6)	6452(3)	49(1)
C(37)	7449(7)	11382(7)	6073(4)	69(2)
Cl(1)	8762(1)	3420(1)	574(1)	51(1)
O(12)	9693(5)	2739(7)	729(4)	90(2)
O(13)	8816(7)	4300(9)	1163(5)	113(3)
O(14)	8808(11)	4105(9)	-133(5)	137(4)
O(15)	7830(6)	2745(10)	321(7)	142(4)
C(41)	5926(8)	5970(11)	4364(5)	88(3)
Cl(2)	5750(7)	4839(5)	4974(3)	145(3)
Cl(3)	5378(5)	7363(4)	4599(2)	106(2)
Cl(4)	7304(4)	6402(12)	4505(3)	180(5)
Cl(2A)	5424(14)	5620(30)	5083(10)	173(9)
Cl(3A)	6340(30)	7379(17)	4531(8)	173(10)
Cl(4A)	6970(11)	5030(30)	4368(11)	168(8)
C(42)	400(30)	5010(60)	5790(40)	116(10)
Cl(5)	-720(30)	4000(30)	5558(19)	121(9)
Cl(6)	830(40)	5610(40)	6770(20)	181(13)
Cl(7)	1470(19)	4320(30)	5529(19)	112(7)
C(42A)	690(20)	4920(20)	5880(18)	116(10)
Cl(5A)	-618(11)	4467(17)	5864(9)	127(5)
Cl(6A)	516(10)	6469(12)	5641(8)	138(4)
Cl(7A)	963(18)	4190(20)	5060(11)	176(7)
N(3)	2260(20)	4360(20)	7483(19)	136(9)
C(51)	2260(30)	5250(40)	7710(20)	126(9)
C(52)	2240(40)	6350(30)	8110(20)	159(13)

Table 122. Bond lengths [Å] for s18phar1.

N(1)-C(5)	1.350(11)
N(1)-C(1)	1.428(10)
N(1)-C(6)	1.430(7)
N(2)-C(22)	1.497(7)
N(2)-C(19)	1.520(6)
N(2)-C(20)	1.522(7)
N(2)-H(2)	1.0000
O(1)-C(1)	1.180(10)
O(2)-C(5)	1.228(11)
O(3)-C(12)	1.204(7)
O(4)-C(12)	1.334(7)
O(4)-C(13)	1.442(8)
O(5)-C(17)	1.432(8)
O(5)-C(16)	1.433(7)
O(6)-C(18)	1.422(7)
O(6)-H(6)	0.8400
O(7)-C(26)	1.428(9)
O(7)-C(25)	1.431(8)
O(8)-C(32)	1.407(8)
O(8)-C(31)	1.443(7)
O(9)-C(34)	1.425(7)
O(9)-H(9)	0.8400
O(10)-C(36)	1.407(8)
O(10)-C(37)	1.412(9)
C(1)-C(2)	1.519(10)
C(2)-C(3)	1.496(15)
C(2)-C(4)	1.509(15)
C(2)-H(2A)	1.0000
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(4)-C(5)	1.512(11)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(6)-C(7)	1.362(9)
C(6)-C(11)	1.404(8)
C(7)-C(8)	1.395(9)

C(7)-H(7)	0.9500
C(8)-C(9)	1.383(10)
C(8)-H(8)	0.9500
C(9)-C(10)	1.390(10)
C(9)-H(9A)	0.9500
C(10)-C(11)	1.395(8)
C(10)-H(10)	0.9500
C(11)-C(12)	1.485(8)
C(13)-C(14)	1.534(8)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(22)	1.541(8)
C(14)-C(15)	1.555(7)
C(14)-C(23)	1.561(10)
C(15)-C(16)	1.535(9)
C(15)-C(27)	1.557(7)
C(15)-H(15)	1.0000
C(16)-C(18)	1.560(8)
C(16)-H(16)	1.0000
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-C(19)	1.534(7)
C(18)-C(34)	1.558(7)
C(19)-C(27)	1.530(7)
C(19)-H(19)	1.0000
C(20)-C(21)	1.505(8)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-C(24)	1.505(11)
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-C(25)	1.517(9)
C(24)-H(24A)	0.9900

C(24)-H(24B)	0.9900
C(25)-C(27)	1.559(8)
C(25)-H(25)	1.0000
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-C(28)	1.556(7)
C(28)-C(35)	1.548(9)
C(28)-C(29)	1.576(8)
C(28)-H(28)	1.0000
C(29)-C(30)	1.540(8)
C(29)-H(29A)	0.9900
C(29)-H(29B)	0.9900
C(30)-C(36)	1.527(8)
C(30)-C(31)	1.532(7)
C(30)-H(30)	1.0000
C(31)-C(33)	1.541(8)
C(31)-H(31)	1.0000
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-C(34)	1.541(8)
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(34)-C(35)	1.552(8)
C(35)-C(36)	1.536(8)
C(35)-H(35)	1.0000
C(36)-H(36)	1.0000
C(37)-H(37A)	0.9800
C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800
Cl(1)-O(15)	1.368(7)
Cl(1)-O(12)	1.371(5)
Cl(1)-O(13)	1.403(7)
Cl(1)-O(14)	1.471(10)
C(41)-Cl(3A)	1.63(2)
C(41)-Cl(2A)	1.635(18)
C(41)-Cl(4A)	1.693(18)
C(41)-Cl(2)	1.700(13)
C(41)-Cl(3)	1.781(12)

C(41)-Cl(4)	1.785(12)
C(41)-H(41)	1.0000
C(41)-H(41A)	1.0000
C(42)-Cl(7)	1.75(3)
C(42)-Cl(6)	1.76(3)
C(42)-Cl(5)	1.77(3)
C(42)-H(42)	1.0000
C(42A)-Cl(6A)	1.74(2)
C(42A)-Cl(5A)	1.76(2)
C(42A)-Cl(7A)	1.78(2)
C(42A)-H(42A)	1.0000
N(3)-C(51)	1.05(4)
C(51)-C(52)	1.40(5)
C(52)-H(52A)	0.9800
C(52)-H(52B)	0.9800
C(52)-H(52C)	0.9800

Table 123. Bond angles [°] for s18phar1.

C(5)-N(1)-C(1)	113.7(6)
C(5)-N(1)-C(6)	123.4(6)
C(1)-N(1)-C(6)	122.9(6)
C(22)-N(2)-C(19)	113.6(4)
C(22)-N(2)-C(20)	109.6(4)
C(19)-N(2)-C(20)	116.1(4)
C(22)-N(2)-H(2)	105.5
C(19)-N(2)-H(2)	105.5
C(20)-N(2)-H(2)	105.5
C(12)-O(4)-C(13)	116.8(5)
C(17)-O(5)-C(16)	112.7(5)
C(18)-O(6)-H(6)	109.5
C(26)-O(7)-C(25)	115.8(6)
C(32)-O(8)-C(31)	112.0(5)
C(34)-O(9)-H(9)	109.5
C(36)-O(10)-C(37)	112.9(6)
O(1)-C(1)-N(1)	124.4(6)
O(1)-C(1)-C(2)	128.2(7)
N(1)-C(1)-C(2)	107.5(7)

C(3)-C(2)-C(4)	117.6(9)
C(3)-C(2)-C(1)	110.6(8)
C(4)-C(2)-C(1)	103.6(7)
C(3)-C(2)-H(2A)	108.2
C(4)-C(2)-H(2A)	108.2
C(1)-C(2)-H(2A)	108.2
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(2)-C(4)-C(5)	107.6(7)
C(2)-C(4)-H(4A)	110.2
C(5)-C(4)-H(4A)	110.2
C(2)-C(4)-H(4B)	110.2
C(5)-C(4)-H(4B)	110.2
H(4A)-C(4)-H(4B)	108.5
O(2)-C(5)-N(1)	124.0(7)
O(2)-C(5)-C(4)	128.6(8)
N(1)-C(5)-C(4)	107.4(8)
C(7)-C(6)-C(11)	121.7(6)
C(7)-C(6)-N(1)	119.0(5)
C(11)-C(6)-N(1)	119.3(5)
C(6)-C(7)-C(8)	120.5(6)
C(6)-C(7)-H(7)	119.7
C(8)-C(7)-H(7)	119.7
C(9)-C(8)-C(7)	118.9(6)
C(9)-C(8)-H(8)	120.5
C(7)-C(8)-H(8)	120.5
C(8)-C(9)-C(10)	120.5(6)
C(8)-C(9)-H(9A)	119.7
C(10)-C(9)-H(9A)	119.7
C(9)-C(10)-C(11)	120.8(6)
C(9)-C(10)-H(10)	119.6
C(11)-C(10)-H(10)	119.6
C(10)-C(11)-C(6)	117.5(5)
C(10)-C(11)-C(12)	120.4(5)
C(6)-C(11)-C(12)	122.0(5)

O(3)-C(12)-O(4)	123.1(5)
O(3)-C(12)-C(11)	126.4(5)
O(4)-C(12)-C(11)	110.5(5)
O(4)-C(13)-C(14)	106.2(5)
O(4)-C(13)-H(13A)	110.5
C(14)-C(13)-H(13A)	110.5
O(4)-C(13)-H(13B)	110.5
C(14)-C(13)-H(13B)	110.5
H(13A)-C(13)-H(13B)	108.7
C(13)-C(14)-C(22)	106.5(5)
C(13)-C(14)-C(15)	110.2(5)
C(22)-C(14)-C(15)	108.9(5)
C(13)-C(14)-C(23)	107.4(5)
C(22)-C(14)-C(23)	112.4(5)
C(15)-C(14)-C(23)	111.3(5)
C(16)-C(15)-C(14)	109.6(5)
C(16)-C(15)-C(27)	104.8(4)
C(14)-C(15)-C(27)	107.7(4)
C(16)-C(15)-H(15)	111.5
C(14)-C(15)-H(15)	111.5
C(27)-C(15)-H(15)	111.5
O(5)-C(16)-C(15)	113.8(5)
O(5)-C(16)-C(18)	111.9(5)
C(15)-C(16)-C(18)	105.1(4)
O(5)-C(16)-H(16)	108.6
C(15)-C(16)-H(16)	108.6
C(18)-C(16)-H(16)	108.6
O(5)-C(17)-H(17A)	109.5
O(5)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
O(5)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
O(6)-C(18)-C(19)	111.0(4)
O(6)-C(18)-C(34)	109.2(5)
C(19)-C(18)-C(34)	108.8(4)
O(6)-C(18)-C(16)	111.5(5)
C(19)-C(18)-C(16)	102.9(4)
C(34)-C(18)-C(16)	113.2(4)

N(2)-C(19)-C(27)	110.2(4)
N(2)-C(19)-C(18)	114.4(4)
C(27)-C(19)-C(18)	102.0(4)
N(2)-C(19)-H(19)	110.0
C(27)-C(19)-H(19)	110.0
C(18)-C(19)-H(19)	110.0
C(21)-C(20)-N(2)	113.8(5)
C(21)-C(20)-H(20A)	108.8
N(2)-C(20)-H(20A)	108.8
C(21)-C(20)-H(20B)	108.8
N(2)-C(20)-H(20B)	108.8
H(20A)-C(20)-H(20B)	107.7
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
N(2)-C(22)-C(14)	111.5(5)
N(2)-C(22)-H(22A)	109.3
C(14)-C(22)-H(22A)	109.3
N(2)-C(22)-H(22B)	109.3
C(14)-C(22)-H(22B)	109.3
H(22A)-C(22)-H(22B)	108.0
C(24)-C(23)-C(14)	112.9(5)
C(24)-C(23)-H(23A)	109.0
C(14)-C(23)-H(23A)	109.0
C(24)-C(23)-H(23B)	109.0
C(14)-C(23)-H(23B)	109.0
H(23A)-C(23)-H(23B)	107.8
C(23)-C(24)-C(25)	112.0(6)
C(23)-C(24)-H(24A)	109.2
C(25)-C(24)-H(24A)	109.2
C(23)-C(24)-H(24B)	109.2
C(25)-C(24)-H(24B)	109.2
H(24A)-C(24)-H(24B)	107.9
O(7)-C(25)-C(24)	111.5(5)
O(7)-C(25)-C(27)	107.7(5)
C(24)-C(25)-C(27)	110.7(5)

O(7)-C(25)-H(25)	109.0
C(24)-C(25)-H(25)	109.0
C(27)-C(25)-H(25)	109.0
O(7)-C(26)-H(26A)	109.5
O(7)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
O(7)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(19)-C(27)-C(28)	107.1(4)
C(19)-C(27)-C(15)	98.1(4)
C(28)-C(27)-C(15)	114.1(4)
C(19)-C(27)-C(25)	117.8(5)
C(28)-C(27)-C(25)	106.1(5)
C(15)-C(27)-C(25)	113.6(5)
C(35)-C(28)-C(27)	118.9(5)
C(35)-C(28)-C(29)	104.5(5)
C(27)-C(28)-C(29)	111.7(5)
C(35)-C(28)-H(28)	107.1
C(27)-C(28)-H(28)	107.1
C(29)-C(28)-H(28)	107.1
C(30)-C(29)-C(28)	105.3(5)
C(30)-C(29)-H(29A)	110.7
C(28)-C(29)-H(29A)	110.7
C(30)-C(29)-H(29B)	110.7
C(28)-C(29)-H(29B)	110.7
H(29A)-C(29)-H(29B)	108.8
C(36)-C(30)-C(31)	112.1(5)
C(36)-C(30)-C(29)	100.5(5)
C(31)-C(30)-C(29)	111.3(5)
C(36)-C(30)-H(30)	110.8
C(31)-C(30)-H(30)	110.8
C(29)-C(30)-H(30)	110.8
O(8)-C(31)-C(30)	106.7(4)
O(8)-C(31)-C(33)	109.5(5)
C(30)-C(31)-C(33)	113.8(4)
O(8)-C(31)-H(31)	108.9
C(30)-C(31)-H(31)	108.9
C(33)-C(31)-H(31)	108.9

O(8)-C(32)-H(32A)	109.5
O(8)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
O(8)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(31)-C(33)-C(34)	117.9(5)
C(31)-C(33)-H(33A)	107.8
C(34)-C(33)-H(33A)	107.8
C(31)-C(33)-H(33B)	107.8
C(34)-C(33)-H(33B)	107.8
H(33A)-C(33)-H(33B)	107.2
O(9)-C(34)-C(33)	104.8(5)
O(9)-C(34)-C(35)	110.7(4)
C(33)-C(34)-C(35)	112.2(5)
O(9)-C(34)-C(18)	107.4(4)
C(33)-C(34)-C(18)	112.4(4)
C(35)-C(34)-C(18)	109.2(5)
C(36)-C(35)-C(28)	101.5(5)
C(36)-C(35)-C(34)	111.3(5)
C(28)-C(35)-C(34)	113.1(4)
C(36)-C(35)-H(35)	110.2
C(28)-C(35)-H(35)	110.2
C(34)-C(35)-H(35)	110.2
O(10)-C(36)-C(30)	116.9(5)
O(10)-C(36)-C(35)	112.0(5)
C(30)-C(36)-C(35)	101.4(4)
O(10)-C(36)-H(36)	108.7
C(30)-C(36)-H(36)	108.7
C(35)-C(36)-H(36)	108.7
O(10)-C(37)-H(37A)	109.5
O(10)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
O(10)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
O(15)-Cl(1)-O(12)	113.9(6)
O(15)-Cl(1)-O(13)	117.0(5)
O(12)-Cl(1)-O(13)	112.4(5)

O(15)-Cl(1)-O(14)	104.8(7)
O(12)-Cl(1)-O(14)	100.9(6)
O(13)-Cl(1)-O(14)	105.8(6)
Cl(3A)-C(41)-Cl(2A)	105.5(15)
Cl(3A)-C(41)-Cl(4A)	111.0(16)
Cl(2A)-C(41)-Cl(4A)	110.9(15)
Cl(2)-C(41)-Cl(3)	109.7(6)
Cl(2)-C(41)-Cl(4)	115.0(7)
Cl(3)-C(41)-Cl(4)	101.0(7)
Cl(2)-C(41)-H(41)	110.2
Cl(3)-C(41)-H(41)	110.2
Cl(4)-C(41)-H(41)	110.2
Cl(3A)-C(41)-H(41A)	109.8
Cl(2A)-C(41)-H(41A)	109.8
Cl(4A)-C(41)-H(41A)	109.8
Cl(7)-C(42)-Cl(6)	112(3)
Cl(7)-C(42)-Cl(5)	109(3)
Cl(6)-C(42)-Cl(5)	117(4)
Cl(7)-C(42)-H(42)	106.0
Cl(6)-C(42)-H(42)	106.0
Cl(5)-C(42)-H(42)	106.0
Cl(6A)-C(42A)-Cl(5A)	102.5(16)
Cl(6A)-C(42A)-Cl(7A)	106.6(17)
Cl(5A)-C(42A)-Cl(7A)	106.5(16)
Cl(6A)-C(42A)-H(42A)	113.5
Cl(5A)-C(42A)-H(42A)	113.5
Cl(7A)-C(42A)-H(42A)	113.5
N(3)-C(51)-C(52)	172(4)
C(51)-C(52)-H(52A)	109.5
C(51)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5
C(51)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5

Table 124. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for s18phar1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	38(2)	64(3)	58(3)	8(2)	19(2)	-13(2)
N(2)	43(2)	41(2)	36(2)	6(2)	5(2)	-9(2)
O(1)	60(3)	82(4)	80(3)	16(3)	32(2)	6(3)
O(2)	70(3)	83(4)	91(4)	-22(3)	24(3)	-30(3)
O(3)	52(2)	59(3)	48(2)	5(2)	9(2)	-19(2)
O(4)	80(3)	56(3)	43(2)	1(2)	3(2)	-33(2)
O(5)	47(2)	61(3)	48(2)	8(2)	-9(2)	-13(2)
O(6)	42(2)	55(2)	50(2)	-1(2)	18(2)	-3(2)
O(7)	49(2)	47(2)	71(3)	5(2)	11(2)	7(2)
O(8)	53(2)	37(2)	49(2)	1(2)	3(2)	-10(2)
O(9)	42(2)	52(2)	63(2)	13(2)	2(2)	7(2)
O(10)	70(3)	45(2)	51(2)	13(2)	2(2)	-8(2)
C(1)	39(3)	80(5)	61(4)	19(4)	21(3)	-1(3)
C(2)	48(3)	93(6)	78(5)	17(4)	16(3)	-7(4)
C(3)	89(7)	176(14)	86(6)	46(8)	14(5)	1(8)
C(4)	48(4)	132(9)	74(5)	-6(5)	1(3)	-25(5)
C(5)	54(3)	75(5)	73(4)	1(4)	23(3)	-20(4)
C(6)	37(2)	56(3)	53(3)	3(3)	22(2)	-8(2)
C(7)	50(3)	57(4)	58(3)	4(3)	28(3)	-4(3)
C(8)	52(3)	69(4)	49(3)	7(3)	20(3)	0(3)
C(9)	49(3)	69(4)	48(3)	-2(3)	14(2)	-4(3)
C(10)	41(3)	59(4)	44(3)	-7(3)	14(2)	-10(3)
C(11)	39(2)	45(3)	45(3)	-4(2)	16(2)	-6(2)
C(12)	42(2)	42(3)	48(3)	-5(2)	21(2)	-10(2)
C(13)	68(4)	53(3)	46(3)	1(3)	5(3)	-24(3)
C(14)	60(3)	38(3)	43(3)	1(2)	10(2)	-15(3)
C(15)	54(3)	41(3)	34(2)	0(2)	6(2)	-11(2)
C(16)	44(3)	47(3)	41(2)	7(2)	5(2)	-9(2)
C(17)	57(4)	90(6)	68(4)	8(4)	-12(3)	-30(4)
C(18)	39(2)	44(3)	37(2)	3(2)	5(2)	-1(2)
C(19)	41(2)	33(2)	35(2)	4(2)	5(2)	-5(2)
C(20)	56(3)	50(3)	35(2)	2(2)	5(2)	-16(3)
C(21)	59(3)	69(4)	41(3)	-4(3)	5(2)	-22(3)
C(22)	53(3)	44(3)	43(3)	6(2)	7(2)	-16(3)

C(23)	84(4)	32(3)	61(3)	-1(3)	18(3)	-7(3)
C(24)	78(4)	39(3)	65(4)	-3(3)	23(3)	1(3)
C(25)	58(3)	40(3)	65(3)	0(3)	20(3)	1(3)
C(26)	51(4)	66(5)	124(7)	11(5)	15(4)	11(4)
C(27)	48(3)	33(2)	42(2)	2(2)	11(2)	-4(2)
C(28)	56(3)	39(3)	38(2)	-2(2)	16(2)	-8(2)
C(29)	51(3)	39(3)	50(3)	-3(2)	21(2)	-7(2)
C(30)	49(3)	40(3)	43(3)	3(2)	16(2)	-8(2)
C(31)	48(3)	34(3)	37(2)	0(2)	5(2)	-5(2)
C(32)	60(3)	43(3)	50(3)	-4(3)	1(3)	-3(3)
C(33)	49(3)	39(3)	38(2)	0(2)	6(2)	0(2)
C(34)	39(2)	39(3)	43(3)	5(2)	5(2)	1(2)
C(35)	52(3)	43(3)	34(2)	3(2)	4(2)	-10(3)
C(36)	63(3)	44(3)	35(2)	6(2)	9(2)	-9(3)
C(37)	93(5)	54(4)	53(3)	13(3)	11(3)	-16(4)
Cl(1)	36(1)	52(1)	59(1)	-10(1)	5(1)	7(1)
O(12)	57(3)	101(5)	104(4)	-18(4)	14(3)	33(3)
O(13)	98(5)	138(7)	108(5)	-60(5)	40(4)	2(5)
O(14)	217(11)	95(6)	82(5)	20(4)	18(6)	33(7)
O(15)	61(4)	166(9)	196(10)	-92(8)	36(5)	-50(5)
C(41)	93(6)	112(8)	50(4)	-16(4)	7(4)	10(6)
Cl(2)	227(7)	100(3)	59(2)	9(2)	-32(3)	-18(4)
Cl(3)	131(3)	108(3)	75(2)	-40(2)	26(2)	-2(3)
Cl(4)	83(2)	375(15)	87(3)	30(5)	33(2)	7(5)
Cl(2A)	105(8)	320(20)	97(8)	2(13)	29(6)	-62(13)
Cl(3A)	270(20)	116(10)	86(7)	-30(7)	-11(10)	-41(13)
Cl(4A)	71(6)	250(20)	154(11)	-61(12)	-11(6)	42(9)
C(42)	109(12)	124(12)	119(12)	13(8)	38(9)	12(8)
Cl(5)	113(15)	132(18)	117(17)	30(14)	36(13)	32(14)
Cl(6)	230(20)	170(20)	158(18)	35(18)	82(18)	58(19)
Cl(7)	96(11)	102(12)	161(18)	2(14)	74(12)	-11(10)
C(42A)	109(12)	124(12)	119(12)	13(8)	38(9)	12(8)
Cl(5A)	89(6)	178(13)	130(9)	21(8)	59(6)	36(7)
Cl(6A)	131(7)	129(8)	143(8)	-13(7)	27(6)	24(7)
Cl(7A)	221(15)	195(14)	165(11)	17(11)	140(11)	36(12)
N(3)	160(20)	85(13)	180(20)	46(16)	90(20)	26(15)
C(51)	124(13)	136(14)	127(13)	-14(11)	51(10)	-11(11)
C(52)	220(20)	103(18)	170(20)	14(17)	77(19)	-21(18)

Table 125. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for s18phar1.

	x	y	z	U(eq)
H(2)	7954	5629	8983	49
H(6)	5019	7919	8346	72
H(9)	4780	8890	6933	84
H(2A)	691	616	7690	88
H(3A)	1394	1800	6500	179
H(3B)	854	2521	7075	179
H(3C)	165	1521	6467	179
H(4A)	1594	-404	6611	106
H(4B)	1096	-1095	7226	106
H(7)	3793	-1129	9446	63
H(8)	5481	-1080	10439	66
H(9A)	6723	456	10404	67
H(10)	6338	1845	9354	57
H(13A)	4558	4442	7579	70
H(13B)	5060	3465	7106	70
H(15)	6002	5329	6692	54
H(16)	4920	6265	7635	55
H(17A)	3403	6716	5724	118
H(17B)	3304	6440	6591	118
H(17C)	3995	5547	6211	118
H(19)	7814	7596	8399	46
H(20A)	6603	7016	9660	58
H(20B)	7478	6013	10102	58
H(21A)	7921	8384	9633	88
H(21B)	8849	7363	9874	88
H(21C)	8287	7832	10515	88
H(22A)	5686	5531	8684	58
H(22B)	6552	4494	9086	58
H(23A)	7612	3518	8425	72
H(23B)	6838	2874	7644	72
H(24A)	7499	4063	6824	73
H(24B)	8531	3540	7499	73
H(25)	8748	5649	7275	65

H(26A)	9962	4125	8411	124
H(26B)	10338	4940	9201	124
H(26C)	10455	5459	8382	124
H(28)	7388	6822	6375	52
H(29A)	9031	7594	7701	55
H(29B)	9034	7644	6789	55
H(30)	9009	9709	7015	52
H(31)	8699	9160	8368	50
H(32A)	9267	12098	8922	82
H(32B)	9460	10699	9193	82
H(32C)	8278	11290	9010	82
H(33A)	6781	10536	7771	52
H(33B)	7074	9582	8487	52
H(35)	6019	8153	6222	54
H(36)	7510	9073	5953	58
H(37A)	7680	11068	5630	104
H(37B)	8089	11592	6518	104
H(37C)	7001	12113	5901	104
H(41)	5567	5746	3795	106
H(41A)	5347	5912	3840	106
H(42)	171	5729	5431	140
H(42A)	1257	4762	6400	140
H(52A)	2968	6725	8252	238
H(52B)	2044	6193	8593	238
H(52C)	1715	6910	7763	238

Table 126. Torsion angles [°] for s18phar1.

C(5)-N(1)-C(1)-O(1)	-175.2(6)
C(6)-N(1)-C(1)-O(1)	2.7(9)
C(5)-N(1)-C(1)-C(2)	5.3(7)
C(6)-N(1)-C(1)-C(2)	-176.8(5)
O(1)-C(1)-C(2)-C(3)	48.1(12)
N(1)-C(1)-C(2)-C(3)	-132.4(8)
O(1)-C(1)-C(2)-C(4)	175.0(7)
N(1)-C(1)-C(2)-C(4)	-5.5(8)
C(3)-C(2)-C(4)-C(5)	126.4(9)
C(1)-C(2)-C(4)-C(5)	4.1(9)

C(1)-N(1)-C(5)-O(2)	176.8(7)
C(6)-N(1)-C(5)-O(2)	-1.1(10)
C(1)-N(1)-C(5)-C(4)	-2.5(8)
C(6)-N(1)-C(5)-C(4)	179.6(6)
C(2)-C(4)-C(5)-O(2)	179.5(8)
C(2)-C(4)-C(5)-N(1)	-1.3(9)
C(5)-N(1)-C(6)-C(7)	-66.7(8)
C(1)-N(1)-C(6)-C(7)	115.5(7)
C(5)-N(1)-C(6)-C(11)	115.2(7)
C(1)-N(1)-C(6)-C(11)	-62.5(7)
C(11)-C(6)-C(7)-C(8)	-1.1(10)
N(1)-C(6)-C(7)-C(8)	-179.1(6)
C(6)-C(7)-C(8)-C(9)	2.5(10)
C(7)-C(8)-C(9)-C(10)	-2.0(10)
C(8)-C(9)-C(10)-C(11)	0.2(10)
C(9)-C(10)-C(11)-C(6)	1.2(9)
C(9)-C(10)-C(11)-C(12)	-176.1(6)
C(7)-C(6)-C(11)-C(10)	-0.7(9)
N(1)-C(6)-C(11)-C(10)	177.2(5)
C(7)-C(6)-C(11)-C(12)	176.4(5)
N(1)-C(6)-C(11)-C(12)	-5.6(8)
C(13)-O(4)-C(12)-O(3)	-0.2(9)
C(13)-O(4)-C(12)-C(11)	178.0(6)
C(10)-C(11)-C(12)-O(3)	156.2(6)
C(6)-C(11)-C(12)-O(3)	-20.9(9)
C(10)-C(11)-C(12)-O(4)	-21.9(7)
C(6)-C(11)-C(12)-O(4)	161.0(6)
C(12)-O(4)-C(13)-C(14)	-156.7(6)
O(4)-C(13)-C(14)-C(22)	-57.3(7)
O(4)-C(13)-C(14)-C(15)	-175.4(5)
O(4)-C(13)-C(14)-C(23)	63.2(7)
C(13)-C(14)-C(15)-C(16)	69.1(6)
C(22)-C(14)-C(15)-C(16)	-47.4(6)
C(23)-C(14)-C(15)-C(16)	-171.9(5)
C(13)-C(14)-C(15)-C(27)	-177.4(5)
C(22)-C(14)-C(15)-C(27)	66.1(6)
C(23)-C(14)-C(15)-C(27)	-58.4(6)
C(17)-O(5)-C(16)-C(15)	85.2(7)
C(17)-O(5)-C(16)-C(18)	-155.9(6)

C(14)-C(15)-C(16)-O(5)	-139.4(5)
C(27)-C(15)-C(16)-O(5)	105.3(5)
C(14)-C(15)-C(16)-C(18)	97.9(5)
C(27)-C(15)-C(16)-C(18)	-17.5(5)
O(5)-C(16)-C(18)-O(6)	102.5(5)
C(15)-C(16)-C(18)-O(6)	-133.5(5)
O(5)-C(16)-C(18)-C(19)	-138.4(5)
C(15)-C(16)-C(18)-C(19)	-14.4(5)
O(5)-C(16)-C(18)-C(34)	-21.1(7)
C(15)-C(16)-C(18)-C(34)	102.9(5)
C(22)-N(2)-C(19)-C(27)	-59.8(6)
C(20)-N(2)-C(19)-C(27)	171.8(4)
C(22)-N(2)-C(19)-C(18)	54.5(6)
C(20)-N(2)-C(19)-C(18)	-74.0(5)
O(6)-C(18)-C(19)-N(2)	42.1(6)
C(34)-C(18)-C(19)-N(2)	162.4(4)
C(16)-C(18)-C(19)-N(2)	-77.3(5)
O(6)-C(18)-C(19)-C(27)	161.1(4)
C(34)-C(18)-C(19)-C(27)	-78.6(5)
C(16)-C(18)-C(19)-C(27)	41.7(5)
C(22)-N(2)-C(20)-C(21)	-178.7(5)
C(19)-N(2)-C(20)-C(21)	-48.4(7)
C(19)-N(2)-C(22)-C(14)	45.4(7)
C(20)-N(2)-C(22)-C(14)	177.1(5)
C(13)-C(14)-C(22)-N(2)	-167.1(5)
C(15)-C(14)-C(22)-N(2)	-48.2(7)
C(23)-C(14)-C(22)-N(2)	75.7(6)
C(13)-C(14)-C(23)-C(24)	129.9(6)
C(22)-C(14)-C(23)-C(24)	-113.3(6)
C(15)-C(14)-C(23)-C(24)	9.2(7)
C(14)-C(23)-C(24)-C(25)	49.8(8)
C(26)-O(7)-C(25)-C(24)	73.6(8)
C(26)-O(7)-C(25)-C(27)	-164.7(6)
C(23)-C(24)-C(25)-O(7)	62.6(8)
C(23)-C(24)-C(25)-C(27)	-57.3(8)
N(2)-C(19)-C(27)-C(28)	-171.3(4)
C(18)-C(19)-C(27)-C(28)	66.8(5)
N(2)-C(19)-C(27)-C(15)	70.3(5)
C(18)-C(19)-C(27)-C(15)	-51.6(5)

N(2)-C(19)-C(27)-C(25)	-51.9(6)
C(18)-C(19)-C(27)-C(25)	-173.8(5)
C(16)-C(15)-C(27)-C(19)	42.3(5)
C(14)-C(15)-C(27)-C(19)	-74.3(5)
C(16)-C(15)-C(27)-C(28)	-70.6(5)
C(14)-C(15)-C(27)-C(28)	172.8(5)
C(16)-C(15)-C(27)-C(25)	167.6(4)
C(14)-C(15)-C(27)-C(25)	51.0(6)
O(7)-C(25)-C(27)-C(19)	-3.1(7)
C(24)-C(25)-C(27)-C(19)	119.0(6)
O(7)-C(25)-C(27)-C(28)	116.9(5)
C(24)-C(25)-C(27)-C(28)	-121.0(6)
O(7)-C(25)-C(27)-C(15)	-116.9(5)
C(24)-C(25)-C(27)-C(15)	5.1(7)
C(19)-C(27)-C(28)-C(35)	-48.2(6)
C(15)-C(27)-C(28)-C(35)	59.2(7)
C(25)-C(27)-C(28)-C(35)	-174.9(5)
C(19)-C(27)-C(28)-C(29)	73.5(5)
C(15)-C(27)-C(28)-C(29)	-179.1(5)
C(25)-C(27)-C(28)-C(29)	-53.2(6)
C(35)-C(28)-C(29)-C(30)	3.0(5)
C(27)-C(28)-C(29)-C(30)	-126.7(5)
C(28)-C(29)-C(30)-C(36)	-32.3(5)
C(28)-C(29)-C(30)-C(31)	86.6(5)
C(32)-O(8)-C(31)-C(30)	-160.4(5)
C(32)-O(8)-C(31)-C(33)	76.0(6)
C(36)-C(30)-C(31)-O(8)	-101.1(5)
C(29)-C(30)-C(31)-O(8)	147.2(5)
C(36)-C(30)-C(31)-C(33)	19.8(7)
C(29)-C(30)-C(31)-C(33)	-92.0(6)
O(8)-C(31)-C(33)-C(34)	148.3(5)
C(30)-C(31)-C(33)-C(34)	29.0(7)
C(31)-C(33)-C(34)-O(9)	-145.3(5)
C(31)-C(33)-C(34)-C(35)	-25.2(6)
C(31)-C(33)-C(34)-C(18)	98.3(6)
O(6)-C(18)-C(34)-O(9)	-55.2(5)
C(19)-C(18)-C(34)-O(9)	-176.6(4)
C(16)-C(18)-C(34)-O(9)	69.7(6)
O(6)-C(18)-C(34)-C(33)	59.6(6)

C(19)-C(18)-C(34)-C(33)	-61.8(6)
C(16)-C(18)-C(34)-C(33)	-175.6(5)
O(6)-C(18)-C(34)-C(35)	-175.2(4)
C(19)-C(18)-C(34)-C(35)	63.4(5)
C(16)-C(18)-C(34)-C(35)	-50.4(6)
C(27)-C(28)-C(35)-C(36)	152.6(5)
C(29)-C(28)-C(35)-C(36)	27.3(5)
C(27)-C(28)-C(35)-C(34)	33.3(7)
C(29)-C(28)-C(35)-C(34)	-92.0(5)
O(9)-C(34)-C(35)-C(36)	90.3(5)
C(33)-C(34)-C(35)-C(36)	-26.4(6)
C(18)-C(34)-C(35)-C(36)	-151.7(4)
O(9)-C(34)-C(35)-C(28)	-156.2(5)
C(33)-C(34)-C(35)-C(28)	87.1(6)
C(18)-C(34)-C(35)-C(28)	-38.2(6)
C(37)-O(10)-C(36)-C(30)	65.9(7)
C(37)-O(10)-C(36)-C(35)	-177.7(5)
C(31)-C(30)-C(36)-O(10)	53.9(7)
C(29)-C(30)-C(36)-O(10)	172.3(5)
C(31)-C(30)-C(36)-C(35)	-68.2(6)
C(29)-C(30)-C(36)-C(35)	50.2(5)
C(28)-C(35)-C(36)-O(10)	-173.9(4)
C(34)-C(35)-C(36)-O(10)	-53.4(6)
C(28)-C(35)-C(36)-C(30)	-48.5(5)
C(34)-C(35)-C(36)-C(30)	72.1(6)

Table 127. Hydrogen bonds for s18phar1 [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2)...O(7)	1.00	1.83	2.629(7)	134.5
N(2)-H(2)...O(14)#1	1.00	2.32	3.099(10)	133.9
O(6)-H(6)...O(2)#2	0.84	2.22	3.016(7)	157.0
O(9)-H(9)...O(5)	0.84	2.02	2.681(7)	135.0
O(9)-H(9)...Cl(4A^b)#3	0.84	2.97	3.361(15)	110.9

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z+1 #2 x,y+1,z #3 -x+1,y+1/2,-z+1